Florida Onsite Sewage Nitrogen Reduction Strategies Study

Task D.16

Task D Report and STUMOD-FL-HPS User's Guide

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Florida Onsite Sewage Nitrogen Reduction Strategies Study

TASK D.16
DRAFT REPORT

Task D Report and STUMOD-FL-HPS User's Guide

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Table of Contents

List of Tables

List of Figures

1 INTRODUCTION

In Task D for the Florida Onsite Sewage Nitrogen Reduction Strategies (FOSNRS) Study, tools were developed that can be employed by users with various levels of expertise to quantify vadose and groundwater transport from onsite wastewater treatment systems (OWTS). The culmination of Task D is a combined vadose zone and saturated zone model, STUMOD-FL-HPS. This User's Guide, prepared by the Colorado School of Mines (CSM), documents the assumptions, limitations, model development, performance evaluation and parameters affecting nitrogen reduction performance. In addition, a brief description of how to use STUMOD-FL-HPS is provided.

STUMOD-FL-HPS, is a combined aquifer-complex soil model intended to fill the gap that currently exists between end users and complex numerical models by overcoming the limitations in the application of complex models while maintaining an adequate ability to predict contaminant fate and transport. The aquifer module (also referred to as the saturated zone module) uses an analytical contaminant transport equation, a horizontal plane solution (HPS), which is ideally suited for an OWTS by simplifying user input. The previously developed Soil Treatment Unit Model (STUMOD) was modified to Florida conditions (STUMOD-FL) and coupled with the saturated zone module, providing the user with the ability to seamlessly evaluate contaminant transport through the vadose zone and aquifer underlying an OWTS (STUMOD-FL-HPS). The model has been implemented as an Excel Visual Basic Application (Excel VBA) with multiple modules to allow easy implementation by a wide range of users while also providing flexibility to evaluate a wide range of scenarios:

- vadose zone fate and transport (STUMOD-FL),
- saturated zone fate and transport (HPS),
- combined vadose and saturated zone fate and transport (STUMOD-HPS),
- multiple OWTS inputs (Multiple Sites I and Multiple Sites II),
- sensitivity analysis (Sensit), and
- uncertainty analysis (CFD I and CFD II).

The tools developed in Task D are varied with regard to their ability to incorporate complexity, user sophistication, and appropriateness for use. Ideally, the simplest tools are used first and are best used as screening tools to decide if further action is needed. The simplest tools require little user sophistication, but cannot incorporate many of the complexities associated with different OWTS site conditions or pollutant treatment processes (Figure 1.1). The tables estimating nitrogen removal in the Wekiva area (Otis, 2007) are examples of simple tools. While these simple tools may not be appropriate for some decision-making, they do provide indication of whether a treatment goal is likely or unlikely to be met for the specific condition represented. Alternatively, simple-to-use tools provided here offer a similar easy user interface, but incorporate complex and robust evaluation of treatment scenarios and operating conditions. The ouputs from HYDRUS-2D simulations (Task D.7) are an example of the simplest-to-use tools providing the user a visual representation of subsurface behavior in the unsaturated zone (also referred to as the vadose zone) for selected conditions. However, contrary to "simple tools" the treatment information provided by these simulation outputs (graphical and tabular) is based on data generated by numerical models that incorporate complex and robust treatment and operating conditions. Because the choices for representative OWTS conditions are limited, the user must decide how/if their OWTS system fits within the limited treatment estimations displayed by the graphics.

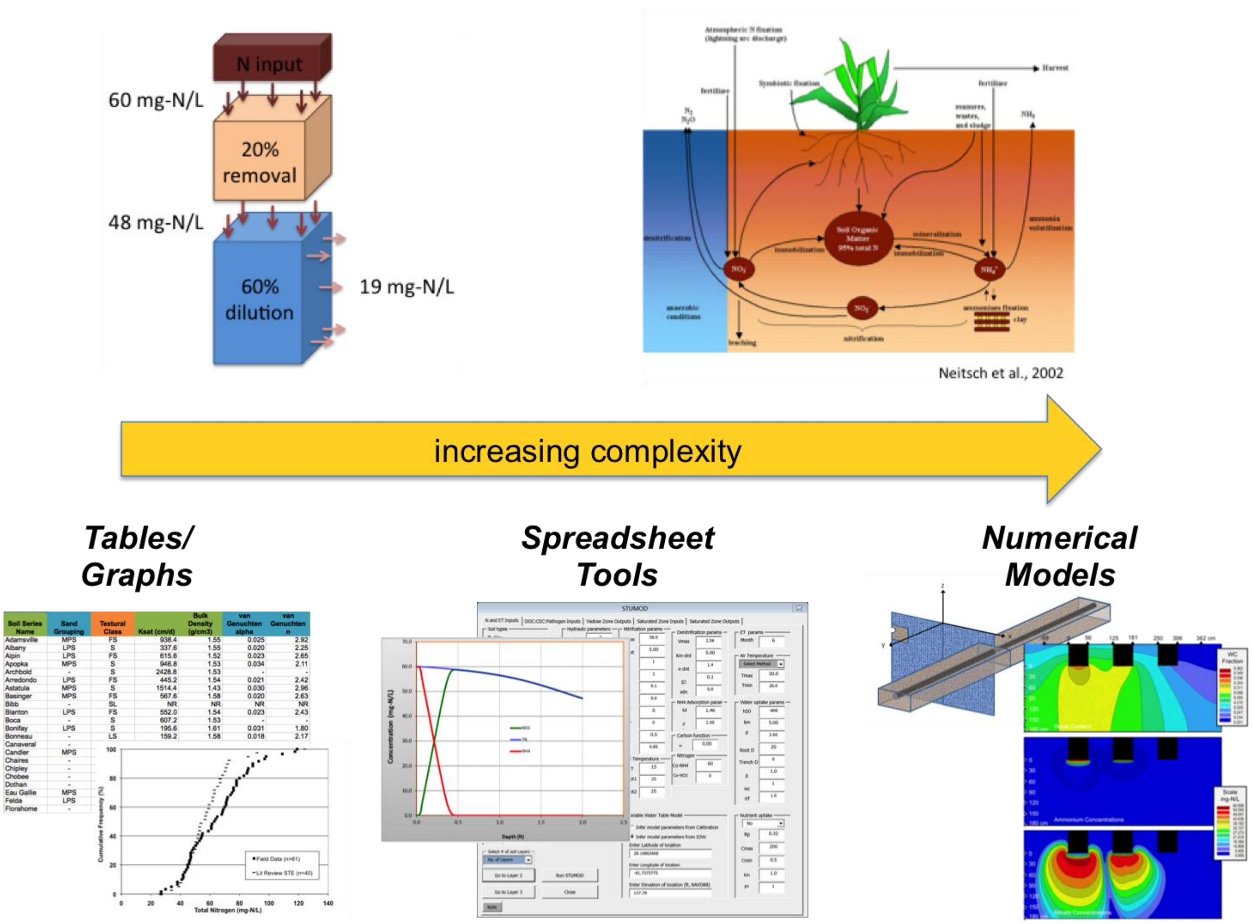

Figure 1.1: Illustration of "Simple" Tools compared to "Simple-to-Use" Tools at various ranges of complexity.

Spreadsheet tools, like STUMOD-FL-HPS, enable treatment estimation for user-specified conditions, but are presented in a simple-to-use format that does not require prior modeling knowledge or lengthy model run times. Of course, achieving these advantages requires that the incorporated treatment processes and operating conditions be simplified. STUMOD-FL-HPS is a spreadsheet tool that enables evaluation of a range of OWTS operating conditions and site conditions. This spreadsheet tool is populated with default values to assist users with limited site knowledge and/or data but incorporates the ability to modify a wide range of input parameters allowing model calibration/corroboration if sufficient data is available.

Nitrogen fate and transport from OWTS in Florida soils and aquifers is known to be complex with various key factors affecting performance such as time variable infiltration, variable nitrogen loading, seasonal precipitation, chain degradation reactions, and subsurface heterogeneities. The factors are so complex that even a numerical model may not be able to account for all these factors simultaneously. STUMOD-FL-HPS was developed as a user-friendly, yet robust, tool to estimate nitrogen transport in soils and aquifers. As the complexity of the OWTS increases or the outcome is more sensitive, a numerical model should be used. Numerical models depending on their robustness, can incorporate an increased level of sophistication regarding subsurface heterogeneity, time variable inputs, or climate.

Use of STUMOD-FL-HPS requires familiarity with spreadsheets and parameter selection, and understanding of hydraulic and treatment mechanisms. Default values are populated into the STUMOD-FL-HPS graphical user interface. However, user-specified inputs can be added instead of default parameters allowing model calibration/corroboration to site-specific data. The output is simulated steady-state performance (i.e., constituent concentration) at the center under the point of effluent application with down gradient transport through the saturated zone. Model outputs provide insight into the behavior of soil treatment, groundwater fate and transport, and quantitative estimations of nitrogen removal as affected by a range of conditions.

2 GOVERNING ASSUMPTIONS FOR STUMOD-FL-HPS

Simple tools can be very helpful for a wide range of common OWTS scenarios. However, there are nearly unlimited possible combinations of OWTS design and operation. Because of limitations in current understanding of mechanisms and processes as well as sufficient data in both frequency and duration, STUMOD-FL-HPS is not sufficient to adequately predict all OWTS configurations and performance. For some high-risk scenarios, the uncertainty in the model predictions may be unacceptable. Tools based on sparse information are no more defensible than tools based on common knowledge without adequate data and in these cases, it must be recognized that more rigorous numerical modeling is required. It is up to the user to decide if the tools developed in Task D are appropriate or if more rigorous modeling/tools are required.

Key governing assumptions include (additional description specific to STUMOD can be found in McCray et al., 2010):

- *Steady state, One-dimensional flow*

  STUMOD-FL-HPS is a 1D vertical steady state model that best represents the long term performance of an OWTS. Variable operating conditions (e.g., changes to effluent quality) or environmental conditions (e.g., precipitation) are not considered.

- *Applied effluent quality*

  Any range of ammonium-nitrogen and nitrate-nitrogen concentrations can be input. STUMOD-FL-HPS does not account for transformations of organic nitrogen.

- *Hydraulic loading rate (HLR)*

  STUMOD-FL-HPS accepts a constant loading rate so an average constant rate is used, time variable HLRs are not supported. The user can specify any HLR less than the saturated hydraulic conductivity of the receiving soil.

- *Effluent delivery method*

  Effluent is applied evenly to a horizontal infiltrative surface with infiltration behaving similarly for each geometry.

- *OWTS geometry*

  A wide range of trench or bed configurations can be simulated. STUMOD-FL is limited to a 1D vertical profile most appropriate for estimating treatment along the centerline below an infiltrative surface. Input from the vadose zone to the HPS module assumes the source zone is the same area as the footprint of OWTS infiltrative surface area.

- *Subsurface heterogeneity*

  Three soil layers including a biomat can be selected with user specified soil textures and thicknesses. Each layer is assumed to have homogenous properties. HPS assumes uniform aquifer properties.

- *Subsurface soil hydraulic properties*

  Hydraulic properties of different soil textures specific to Florida were taken from the Florida Soil Characterization Data Retrieval System (University of Florida, 2007). A look-up table is provided within STUMOD-FL-HPS and additional details are provided in Appendix A.

- *Nitrogen transport and transformation*

  STUMOD-FL development was based on the assumption that ammonium-nitrogen is converted to nitrate-nitrogen, and nitrate-nitrogen is converted to nitrogen gas, based on Monod kinetics, and that the transformations are a function of water content in the soil. It is assumed that sufficient alkalinity is present and that the pH is in a range for sufficient nitrification and denitrification to occur. The cation exchange of ammonium was assumed to be a linear, equilibrium, reversible process and the only nitrogen species that adsorb to soil. First order kinetics are utilized in HPS to simulate the denitrification process in the saturated zone.

- *Carbon function*

  An empirical relationship is based on both the carbon added in the effluent and the carbon in the soil. Biodegradation of the effluent carbon is classified into three categories as: 1) easily biodegradable fraction, 2) a fraction with moderate biodegradation, and 3) a slow biodegrading fraction. Denitrification rates are adjusted based on depth distribution of carbon.

- *Evapotranspiration (ET)*

  ET is assumed to be a function of soil moisture content and root depth relative to the point of infiltration and both nitrate (NO_3) and ammonium (NH_4) are equally available to plants. Plant roots must extend below the infiltrative surface for plant nutrient uptake to occur.

- *Soil and water table interactions*

  The soil moisture content is higher in the capillary fringe and capillary rise is soil texture dependent. The capillary fringe due to its higher moisture content is the zone where relatively higher denitrification occurs depending on availability of carbon.

- *Groundwater transport*

  The analytical HPS solution derived by Galya (1987) is the basis of the saturated zone module. The HPS solution does not consider multidimensional advection, temporally varying boundary conditions, or spatial variation in hydraulic conductivity or denitrification.

- *Cumulative impacts of multiple OWTS*

  There are two different options for simulating the cumulative impacts: 1) one set of averaged parameter values is assumed to be representative of multiple OWTS with average distance to a receiving water body, or 2) each OWTS is assumed to have unique characteristics and distance to receiving water body with mass loading from each OWTS summed at the receiving water body boundary.

3 MODEL DEVELOPMENT AND PARAMETER SELECTION

STUMOD-FL-HPS is a spreadsheet tool that enables evaluation of fate and transport in the vadose and saturated zones from a range of OWTS. Two primary modules form the basis of STUMOD-FL-HPS:

- a vadose zone module based on an analytical solution to the advection dispersion equation (ADE), and
- a saturated zone module also based on an analytical solution to the ADE with a horizontal plane source (HPS).

STUMOD-FL is the vadose zone module and is based on fundamental principles of water movement and contaminant transport using an analytical solution to calculate pressure and moisture content profiles in the vadose zone and a simplification of the general advection dispersion equation (Geza et al., 2009 and 2010). STUMOD was developed at Colorado School of Mines through support from the Water Environment Research Foundation (McCray et al., 2010). STUMOD-FL was adapted to Florida-specific soil and climate data while incorporating ET and high/seasonally variable water tables on nitrogen removal in soil.

The aquifer module incorporates a HPS analytical solution developed for the saturated zone to provide computationally efficient fate and transport of groundwater contaminant plume modeling.

Additional discussion related to the development and corroboration of the vadose module can be found in the FOSNRS Task D.8, D.9, and D.10 reports. Additional discussion related to the development and performance evaluation of the saturated zone module can be found in the FOSNRS Task D.11, D.12, and D.13 reports.

3.1 Vadose Zone Module - STUMOD-FL

STUMOD was developed for transport in the unsaturated zone (McCray et al., 2010). The overall procedure used to calculate nitrogen attenuation in STUMOD is shown in Figure 3.1. First the pressure profile is calculated, then the soil moisture profile is calculated using the pressure profile and soil water retention parameters and saturated hydraulic conductivity.

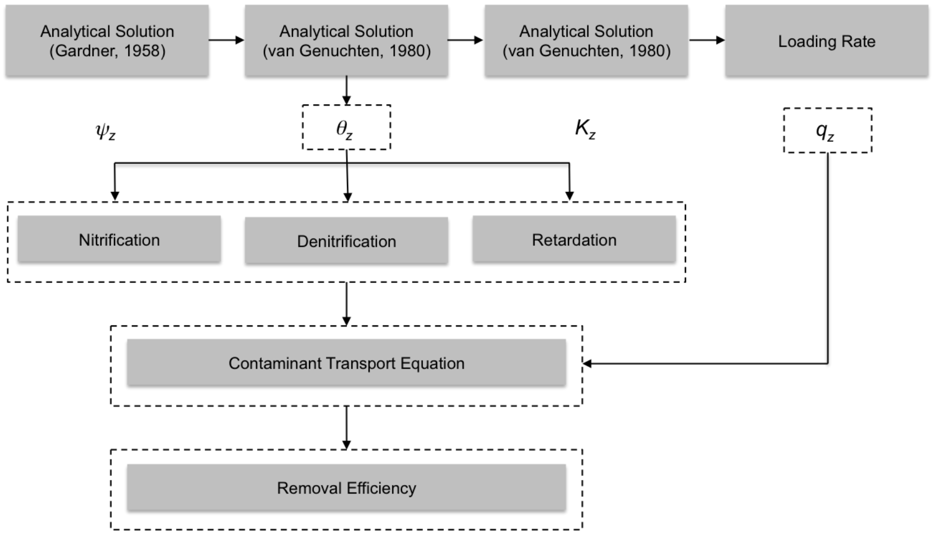

Figure 3.1: Flow chart of nitrogen attenuation incorporated into STUMOD (from McCray et al., 2010).

Vertical flow is assumed to predominate with contaminants transported by advection (the effect of dispersion is ignored). Continuous, steady state effluent application and infiltration is assumed. As the infiltration reaches steady state, the pressure profile or soil moisture profile does not change with time and a steady state concentration with depth is computed based on Monod reaction rates for nitrification and denitrification correlated to the soil moisture profile. The effect of temperature on nitrification and denitrification is also considered. For STUMOD-FL, in addition to a biomat, three soil layers have also been added. STUMOD-FL can accept nitrogen input concentrations as ammonium, nitrate, or a combination of ammonium and nitrate. Ammonium-nitrogen can be removed through both adsorption and denitrification. Nitrate-nitrogen is removed through denitrification. Additional detail can be found in McCray et al., 2010.

3.1.1 OWTS Operating Conditions

There are four key OWTS operating conditions input into STUMOD-FL: 1) effluent quality, 2) HLR, 3) temperature, and 4) soil treatment unit geometry.

STUMOD-FL can accept any range of ammonium-nitrogen and nitrate-nitrogen concentrations. It is generally assumed that about 85 to 90% of the organic nitrogen in raw wastewater is converted to ammonium-nitrogen in the septic tank (APHA, 2005). The concentration of total nitrogen in septic tank effluent (STE) is typically assumed to range from 25 to 125 mg-N/L (Crites and Tchobanoglous, 1998; U.S. EPA, 2002; Lowe et al., 2009). The median total nitrogen concentration ranges between 58 mg-N/L reported in the literature (Lowe et al. 2007) to 64 mg-N/L measured in the field at sites in Colorado, Minnesota, and Florida (Lowe et al., 2009). In the anaerobic septic tank, the conversion of organic-nitrogen to ammonium-nitrogen is rapid and nitrogen remains predominantly as ammonium-nitrogen in STE. The largest fraction of nitrogen in STE is in the form of ammonium-nitrogen with little to no nitrate-nitrogen present. Table 3.1 summarizes the measured concentrations of ammonium-nitrogen as reported by Lowe et al., 2009.

Table 3.1: Ammonium-nitrogen in STE (adapted from Lowe et al., 2009).

		n	Mean	SD	Min	25th Percentile	Median	75th Percentile	Max
All Sites		61	56.4	18.2	25	43	53	68.3	112
Region	Colorado	20	61.1	17.8	28.8	48.7	55.7	75.6	90.6
	Florida	24	55.9	12.9	37.2	42.5	59.4	67.6	76.1
	Minnesota	17	51.6	23.9	24.8	37.6	43.8	53.9	111.7
Season	Fall	15	58.2	24.0	24.8	37.9	52.8	72.9	111.7
	Winter	14	57.0	15.7	38.1	45.9	54.9	67.4	90.6
	Spring	16	50.1	14.3	28.8	38.0	48.3	58.9	80.6
	Summer	16	60.5	17.4	39.2	43.9	58.7	72.3	98.0
Lit Review		26	44	16	19	36	42	52	97

HLR is expressed in STUMOD-FL as cm/d. The HLR can be input as any rate less than the saturated hydraulic conductivity of the receiving soil. STUMOD-FL assumes a constant loading rate applied uniformly over the infiltrative surface. Conversion of design or permit HLRs in gallons per square foot per day (gal/ft^2/d) can easily be expressed in cm/d by multiplying gal/ft^2/d by 4.074 (gal/ft^2/d × 3785 cm^3/gal ÷ 929 ft^2/cm^2 = 4.074 cm)

It is well documented that nitrogen transformation rates generally increase with temperature to a maximum value of about 25°C and decline with additional increasing temperature (Malhi and McGill, 1982; Grundmann et al., 1995; Avrahami et al., 2003). Because soil temperature at depths relevant to OWTS (0.1 to 3 m below surface) can range between 3°C and 25°C (Brady and Weil, 2002) with significant geographical variation, the user can select the average annual soil temperature.

STUMOD-FL is limited to a 1D vertical system. Thus, the module is most appropriate for estimating treatment along the centerline directly below an infiltrative surface and will tend to underestimate the nitrogen removal (over estimate nitrogen concentrations in the soil) resulting in a conservative assessment. The aquifer module (HPS) will accept OWTS trench or bed geometry inputs from STUMOD-FL (Section 3.2.1).

3.1.2 Treatment Depth

In STUMOD-FL, the pressure profile is calculated as a function of the hydraulic loading rate, saturated hydraulic conductivity and Gardner's alpha parameter (α_G). The ultimate goal of calculating pressure head is to calculate the moisture distribution corresponding to the suction head because soil moisture content is a factor considered in the calculation of nitrification and denitrification. Typical ranges for α_G are 0.001 cm^{-1} to 1 cm^{-1} based on the experimentally determined values for several soil textures (Tartakovsky et al., 2003). The default α_G value for different soil types was refined to obtain the soil moisture and pressure distribution corresponding to the soil moisture and pressure profile obtained from a HYDRUS-2D model for identical loading rates.

STUMOD-FL has two options for treatment depth: 1) assume a deep water table, or 2) set the treatment depth equal to the water table depth. For the first case, a deep water table is assumed and there is no capillary effect which would influence the soil moisture profile and denitrification.

For the second option, the treatment depth is assumed to be the top of the water table and soil moisture content in the capillary fringe will have an effect on treatment. In this case, the user can either input a known water table depth or use the water table fluctuation model incorporated to STUMOD-FL to obtain a water table depth. Two methods are applied in the water table fluctuation model implemented within

STUMOD-FL. If the user has access to historical water table fluctuation and precipitation data, the model will conduct an auto-calibration to extract parameter values for the water table fluctuation equation. In the event that the user has precipitation data only, the model will extrapolate parameter values for the water table fluctuation equation stored within STUMOD-FL via inverse distance weighting of groundwater elevation data to the location the user has specified.

3.1.3 Soil Layers and Travel Time

STUMOD-FL considers subsurface heterogeneity by incorporating up to 3 soil layers plus a biomat. If the soil is assumed to have homogenous properties, one layer is selected. To represent heterogeneity, 2 or 3 layers can be selected with the thickness (as defined by the depth to the top of the subsequent layer) and soil texture specified for each layer.

A biomat with a lower permeability relative to the native soil can be added to simulate unsaturated conditions. In the case of no biomat, the user can enter "0" for the thickness or set the hydraulic conductivity equal to the underlying soil. The user can select any biomat thickness, but the literature suggests a typical thickness of 0.5 to 5 cm (Siegrist, 1987; Tyler and Converse, 1994; McKinley and Siegrist, 2010). The biomat properties in STUMOD-FL are then assigned based on literature values (K_{sat}) or assumed to equal the properties of the top soil layer (van Genuchten parameters).

For computational purposes, each soil layer is further divided into several segments. The number of segments in each layer is set to a default value, but can be changed to alter the resolution of the model calculated suction head, soil moisture profile, and nitrogen removal with depth.

The velocity or travel time of effluent in the vadose zone is based on the hydraulic loading rate and soil porosity. This approach is valid assuming the hydraulic loading rate is less than the saturated hydraulic conductivity.

3.1.4 Soil Hydraulic Parameters

When a soil texture for one or more soil layers is selected, the relevant soil hydraulic input parameters for STUMOD-FL are K_{sat}, residual water content (θ_r), water content at saturation (θ_s), and the van Genuchten fitting parameters α and n are automatically populated with default values. While default parameter values are provided in the STUMOD-FL GUI, the user has the option to modify any parameter based on their knowledge of a specific site.

Soil properties were evaluated based on data in the Florida Soil Characterization Data Retrieval System (University of Florida, 2007). Data records were sorted by soil textural classification and then screened for complete data sets (incomplete data sets were removed from further analysis) and data records applicable to depths of less than 5ft below ground surface. All records for a given soil texture (e.g., sandy clay loam, clay, etc.) were then combined and descriptive statistics were evaluated. Median values were then used to represent Florida specific properties for K_{sat}, θ_r, and θ_s. The van Genuchten parameters (α and n) were approximated for the soil moisture curve generated by paring the median reported soil moisture values at each suction head.

Due to the prevalence of sandy soil textures in Florida a hierarchical cluster analysis was conducted with two groupings of sand soil series identified. These two representative groupings of sand soil textures were incorporated into STUMOD-FL as default values for a more permeable sand and a less permeable sand. The more permeable sand is generally characterized by K_{sat} > 500 cm/d, % very fine sand <10%, and total sand fractions of >95%. The less permeable sand is generally characterized by K_{sat} < 500 cm/d, % very fine sand >10%, and total sand fractions of <95%.

Additional detail on determining soil hydraulic parameters is presented in the FOSNRS Tasks D.7 and D.8 reports. A lookup table with default parameters by soil series for the most common Florida soils is included within STUMOD-FL-HPS and Appendix A.

3.1.5 Evapotranspiration (ET) Effects

The effects of ET are expressed in two primary ways: root water uptake and root nutrient uptake. Plant uptake is assumed to be distributed uniformly across the ground surface. Plant roots should extend below the infiltrative surface for nutrient uptake to occur. If plant roots do not extend below the infiltrative surface, plant uptake does not occur. If only a small portion of the root depth extends below the infiltrative surface, plant uptake occurs, but reduced relative to the case where all or a significant portion of the root depth extends below the infiltrative surface.

3.1.5.1 Root Water Uptake

The mathematical form of root water uptake in STUMOD-FL follows equation 3-1 as suggested by Feddes et al. (1978) and Belmans et al. (1983).

$$S(z) = \beta(z)\alpha(h)T_p \tag{3-1}$$

where $\beta(z)$ is the normalized root density distribution (L^{-1}), T_p the potential transpiration rate ($L^3\ L^{-2}\ T^{-1}$), and $\alpha(h)$ is a dimensionless water stress response function ($0 \leq \alpha \leq 1$).

The water stress function, α, is implemented in STUMOD-FL as a smooth, S-shaped reduction function (van Genuchten, 1987) as:

$$\alpha(h) = \frac{1}{1+\left(h/h_{50}\right)^{p_1}} \tag{3-2}$$

where *α(h)* is a dimensionless water stress response function, p_1 is the rate at which the function drops from unity to zero, and h_{50} is the suction at which the transpiration rate is half the potential evapotranspiration, P_T. The soil layer is divided into several segments and the soil water pressure, *h*, is calculated using an analytical approach for each segment (Geza et al., 2010) where the average of the pressure head at the top and bottom of each elemental depth is used to calculate *α(h)* for each layer in equation 3-2.

The potential evapotranspiration is distributed along the soil profile according to a user-defined root density function. A linear decrease in the root density from a maximum at the ground surface to zero at a depth of maximum root depth is implemented. This approach has been implemented in other models including HYDRUS-2D.

3.1.5.2 Root Nutrient Uptake

The approach used in STUMOD-FL is similar to one presented in Šimůnek and Hopmans (2009). STUMOD-FL allows for both passive and active root nutrient uptake. The passive uptake describes the mass flow of dissolved nutrients by plant roots associated with water during transpiration. It is also assumed that the passive uptake is the primary mechanism of supplying plants with nutrients, and that active uptake is initiated only if passive uptake is inadequate. The active uptake includes all other possible nutrient uptake mechanisms, including energy-driven processes against concentration gradients.

A key assumption is that both nitrate and ammonium species are assumed to be equally available to plants. Uptake from each species is proportional to its relative amount in the total mineral nitrogen pool (Johnsson et al., 1987). In STUMOD-FL, the nitrogen demand is mainly supplied by ammonium at shallow depths and nitrate at deeper depths. The modeling approach has a flexible formulation that considers a maximum allowable uptake, c_{max}, Michaelis–Menten constant (K_m) that accounts for the effect of concentration on uptake, and minimum uptake (c_{min}) values that will allow users to vary uptake mechanisms among nutrient types.

3.1.6 Carbon Function

An empirical relationship between carbon availability and denitrification limitation has been incorporated into STUMOD-FL. This empirical relationship is based on both the carbon added in the effluent and the carbon in the soil. The processes are considered in parallel with the maximum carbon (either from effluent or in the soil) controlling the adjustment to denitrification. In this manner, if little carbon is applied in the effluent, the available soil carbon will control the denitrification rate limitation. If significant carbon is applied in the effluent (typical assumption for STE), then the degradation of this effluent carbon will control the limitation on denitrification. Additional detail can be found in the FOSNRS Task D.10 report.

3.1.7 STUMOD-FL Sensitivity

A parameter sensitivity analysis was performed to identify the most relevant model parameters. Thirteen parameters where shown to result in at least a 10% change from the default model output with many of the sensitive parameters in STUMOD-FL being hydraulic parameters (Table 3.2). The pore size distribution parameter (n), saturated soil moisture content (θ_s), air entry pressure (α_{VG}), pressure distribution (α_G), HLR, and hydraulic conductivity (K_s) all produced significant changes in model output during the sensitivity analysis. Denitrification rate and initial effluent concentration were also determined to be influential parameters since the reactions are concentration dependent. Additional detail can be found in the FOSNRS Task D.9 report.

Table 3.2: Order of Sensitive STUMOD-FL Parameters as Determined by Sensitivity Analysis

Normalized % Change in Model Output	Parameter	Parameter Description
100.00 %	n	Parameter n in the soil water retention function
78.09 %	s_{dn}	A threshold relative saturation
74.33 %	T	Soil temperature
74.25 %	V_{max}	Maximum denitrification rate
72.68 %	θ_s	Saturated soil moisture content
61.07 %	HLR	Hydraulic loading rate
60.34 %	C_o NH_4	Effluent ammonium concentration
59.77 %	α_{VG}	Parameter α in the soil water retention function
53.24 %	e_{dnt}	Empirical exponent for denitrification
41.36 %	α_G	Parameter α in Gardner's analytical equation for pressure distribution
29.27 %	sh	Relative saturation for biological process (upper limit)
21.58 %	K_s	Hydraulic conductivity
13.13 %	$kr\ max$	Maximum nitrification rate

3.1.8 STUMOD-FL Uncertainty

An uncertainty analysis was performed where probability-based ranges for model input parameters were used to generate probable model outcomes. In general, higher nitrogen removal can be observed in lower hydraulic loading rates (2 cm/d removal > 5 cm/d removal), in finer grained soil textures (sandy clay loam removal > less permeable sand removal > more permeable sand removal), and with increasing depth (removal at 6 ft is > 4ft > 2 ft > 1ft). The effect of the capillary zone on nitrogen removal was observed due to a relatively significant change in moisture content in sandy soils with a lesser effect observed in sandy clay loam. This is because sandy clay loam has a higher moisture content due its higher water holding capacity regardless of the capillary fringe effect. Additional detail can be found in the FOSNRS Task D.9 report.

3.2 Groundwater Zone Model - HPS

The HPS model is a transient, three-dimensional analytical model capable of simulating advective-dispersive transport and first order reaction (denitrification) in a homogeneous aquifer with uniform horizontal flow. The module assumes the source zone is the same area as the footprint of OWTS source in the vadose module (STUMOD-FL). Thus, the input from the vadose zone to the saturated zone is considered as the average loading per unit area.

The governing equation which describes solute transport in porous media is given by equation 3-3, the advection dispersion equation (ADE) (Fetter, 1999) for a conservative solute. The HPS solution derived by Galya (1987) was utilized because it considers a horizontal mass flux contaminant source. The HPS solution does not require assumptions of a mixing layer beneath the STU or estimation of concentration for the contaminant source, Figure 3.2.

$$\left[\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\right]-\left[\frac{\partial}{\partial x}(v_xC)+\frac{\partial}{\partial y}(v_yC)+\frac{\partial}{\partial y}(v_yC)\right]=\frac{\partial C}{\partial t} \quad (3\text{-}3)$$

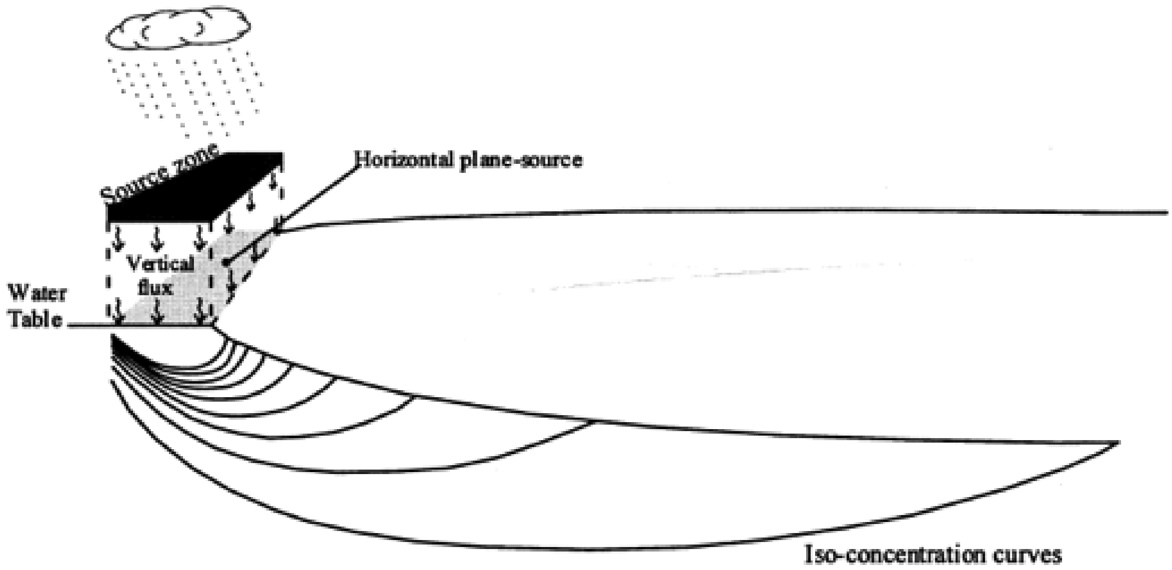

Figure 3.2: Visual representation of the geometry of the HPS model (from Guyonnet, 2001).

The HPS solution was derived by Galya (1987) using the work of Carslaw and Jaeger (1959) and Crank (1975) providing a solution to a modified form of equation 3-3 which considers one dimensional advection and three dimensional dispersion. The solution method is based on a mathematical proof given by Carslaw and Jaeger (1959) which states that a solution to a three dimensional partial differential equation may be derived from individual one dimensional solutions.

3.2.1 OWTS Operating Conditions

The saturated zone module inputs include HLR and OWTS dimensions. As in the vadose zone module, the HLR is the volumetric flow rate applied to the infiltrative surface per day divided by the area of the infiltrative surface. The HLR value is automatically populated by STUMOD-FL. The width and length dimensions refer to the footprint of the infiltrative surface. The latitude and longitude refer to the center of the infiltrative surface and are only utilized if the user chooses to calculate the distance to the point where concentration or mass flux will be evaluated rather than input those data directly.

3.2.2 Aquifer Properties

The porosity and saturated hydraulic conductivity are automatically populated with values from the STUMOD-FL interface if it is run first. The values from STUMOD-FL have been determined based on soil textural classes (Section 3.1.4). The aquifer thickness is the thickness of the saturated zone or the distance from the water table to the first confining unit. An input value of '999' is used to calculate the concentration or mass flux for an aquifer of substantial thickness.

Groundwater seepage velocity is an important parameter in the saturated zone module. Representative saturated hydraulic conductivity and porosity values for several soil textures are available through the STUMOD-FL graphical user interface. The hydraulic gradient, however, must be estimated or calculated directly. If no additional data is available the user may wish to estimate the hydraulic gradient as the average slope of the surrounding land surface. The HPS module has an option to calculate gradient and direction based on the location of three points and hydraulic head at those points. The user may choose to calculate the direction and magnitude of the hydraulic gradient by clicking 'Run Groundwater Model' to calculate the gradient and direction (see Section 4.2.2.1 for more detail). The magnitude and direction of the hydraulic gradient is displayed on the GUI and the direction is plotted on a North arrow imbedded within the GUI. The ability to calculate the direction of the hydraulic gradient independent of a model run is useful because it may indicate to the user that the local direction of flow is oriented differently than what they may have anticipated.

The three dimensional dispersivity values must be input by the user or the user may select to calculate those values based on the longitudinal distance to the observation point. The saturated zone module provides a method whereby the user can choose to allow the model to estimate dispersivity values based on flow length/longitudinal distance. The method was based on a review of studies with reported dispersivity values for surficial sand aquifers similar to those in Florida (Bitsch and Jensen, 1990; Mallants et al., 2000; Sudicky et al., 1983). The estimated dispersivity values are posted to the respective dispersivity input fields once the model is done running to allow the user to evaluate the dispersivity values. The user may alter the estimates after the first model run by unchecking "Estimate Dispersivity" which activates the input fields but does not alter the values.

3.2.3 Contaminant Properties

Nitrate is generally not retarded in the subsurface but the option to change the retardation factor is given to allow a user to the flexibility of modeling the transport of other contaminants in the subsurface, such as ammonium. This option may also be utilized to evaluate the effects of anion exclusion on nitrate transport. Retardation values less than one indicate solutes are traveling faster than the average seepage velocity. This can occur when solutes are restricted to faster moving pore water because of charge repulsion between the soil matrix and the solute (James and Rubin, 1986; McMahon and Thomas, 1974).

First order kinetics are utilized to simulate the denitrification process which is the generally accepted method (McCray et al., 2005). The use of first order kinetics to represent denitrification is a conservative approach. The rate in which denitrification occurs can be selected from a CFD based on either the understanding of or assumptions for the key factors at the site (e.g., soil temperature, carbon content, nitrate-nitrogen concentration, etc.). Figure 3.3 is a CFD of first order denitrification rates for saturated (100% water filled porosity) sands in Florida adapted from Bradley et al. 1992 (temperature corrected to 25°C, Tucholke 2007). The default denitrification rate populated into the saturated zone module was the 25th percentile value of 0.002 d^{-1}. While this rate is conservative (limits denitrification), it was supported by model corroboration. A higher or lower denitrification rate may be appropriate based on site conditions.

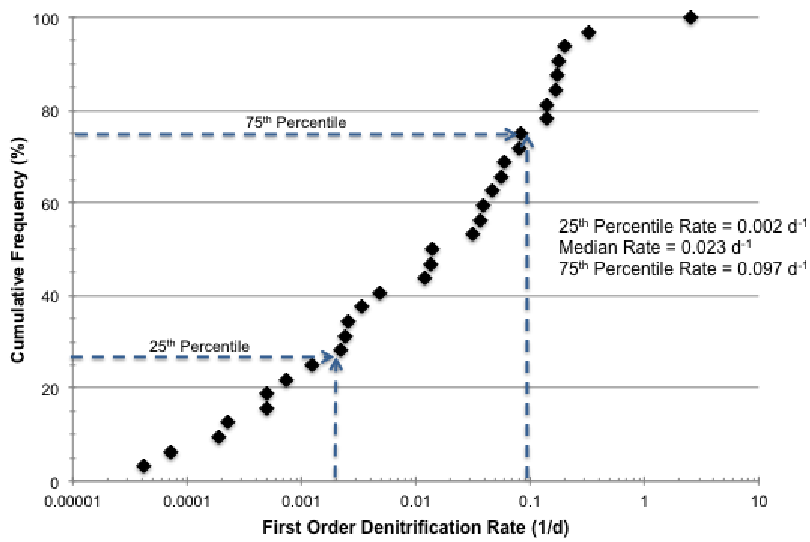

Figure 3.3: Saturated denitrification rates adapted from Bradley et al., 1992 (Tucholke 2007).

Nitrogen concentration is assumed as nitrate (as nitrogen) in the percolate at the water table and in the plume. Nitrate concentration can be calculated at any point within an aquifer receiving STU percolate. The HPS solution assumes a mass flux contaminant source and one dimensional advection. OWTS that use high HLRs may produce mounding of the water table beneath the infiltrative surface promoting transverse advection within the vicinity of the STU. Because the HPS solution considers a mass flux contaminant source plane rather than a constant concentration contaminant source plane, dilution of nitrate by effluent is not accounted for. The transverse advection occurring due to water table mounding and not accounting for dilution will result in over prediction of nitrate concentrations along the plume centerline and under prediction along the plume edges.

Mass flux calculations estimate the mass of nitrate passing through a vertical plane at point down gradient of the source specified by the user (Figure 3.4). The number of rows to columns is determined by the ratio of the plume depth to height. The simulated mass flux of nitrate to a water body is inherently conservative (predicts higher nitrogen mass flux) as the model cannot account for streamlines that do not intersect the water body. In addition, the estimate may be conservative (i.e., less removal) because the model will not account for increased denitrification that may occur within the hyporheic zone. In contrast, mass flux can be underestimated in some situations because denitrification is simulated via first order reaction kinetics. First order reaction kinetics are concentration dependent meaning higher concentrations along the plume centerline result in increased mass removal from the system. Finally, understanding the direction of the hydraulic gradient is critical for estimating potential mass flux. Incorrectly estimating the direction or magnitude of the hydraulic gradient can significantly impact estimates of mass flux for a potential receptor.

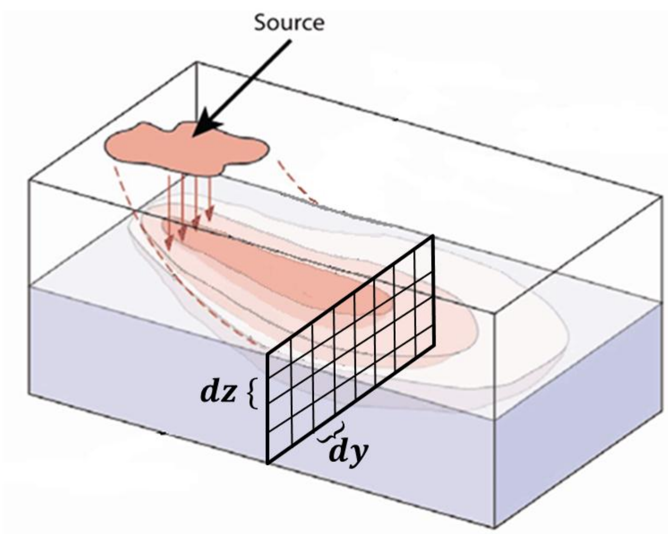

Figure 3.4: Illustration of the saturated zone module mass flux calculated by creating a plane perpendicular to the hydraulic gradient (discretized in N Rows and M Columns).

3.2.4 HPS Sensitivity

Parameter sensitivity analysis indicated that model output was sensitive to retardation, porosity, and the first order denitrification coefficient (Figure 3.5). These results fit with the widely held conceptual model that denitrification is the most critical process in controlling nitrate transport in groundwater. Sensitivity results show that retardation will have a large effect on the calculated concentration because a faster travel time will minimize the amount of nitrate lost to denitrification. Porosity is an important factor controlling seepage velocity such that as porosity decreases the seepage velocity increases and the transport time decreases.

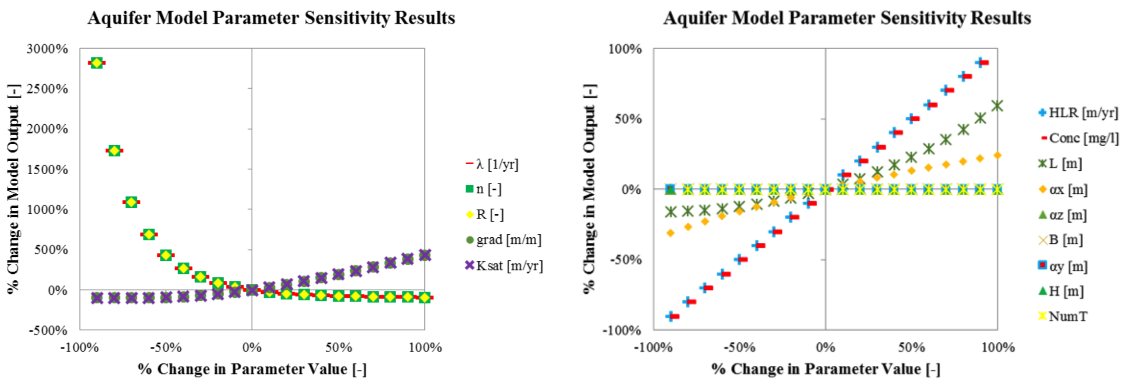

Figure 3.5: HPS sensitivity analysis results

The probable range of denitrification, porosity and retardation values is also important. Denitrification rates ranging over several orders of magnitude are reported in literature (McCray et al., 2005; Tucholke 2007) and because of this, independently measured denitrification rates may not significantly reduce uncertainty in model outputs. Ranges of retardation and porosity in contrast do not vary as widely. Under most conditions nitrate is not retarded eliminating uncertainty related to this parameter while measurements of porosity are commonly within 20% of the actual value greatly reducing model uncertainty.

Hydraulic conductivity and hydraulic gradient were comparatively less sensitive parameters. However, these parameters should be as sensitive also because they act the same way (change the velocity). It is assumed that when either the conductivity or the gradient is reduced, after some point the concentration becomes zero or very low and does not change any more. In this manner, both conductivity and the gradient are so sensitive that the same result (zero concentration) after some point is produced. In addition, due to the large range of possible values these should also be considered critical parameters for the aquifer model. Both hydraulic conductivity and hydraulic gradient control the transport time of solutes when retardation does not occur. Under denitrifying conditions longer transport times may result in a larger mass removal from the aquifer. As a result, in the application of the aquifer model the denitrification rate should be regarded as the most critical parameter followed by hydraulic conductivity, hydraulic gradient and finally retardation and porosity.

3.2.5 HPS Uncertainty

Model uncertainty analysis was conducted for three soil textures (more permeable sand, less permeable sand, and sandy clay loam) supported by STUMOD-FL to provide insight into probable model outcomes. Results indicate that the saturated zone module predicts substantial removal of nitrate for a 200-foot setback distance and that the denitrification parameter significantly controls model output. More specifically, denitrification values greater than the 50th percentile reported by McCray et al., (2005) have a large impact on module output. This conclusion is supported by the alternate uncertainty analysis that was conducted using values equal to or less than the 50th percentile denitrification value. The module outputs for these two uncertainty analyses are significantly different though the only difference was the range of denitrification values that were used. Module output is also dependent on transport parameters such as hydraulic conductivity, hydraulic gradient and porosity. Under conditions of low denitrification, output uncertainty is largely controlled by the physical transport parameters, hydraulic conductivity, hydraulic gradient and porosity.

From a user perspective these results reveal the likelihood of achieving a particular outcome given uncertainty in saturated zone module input parameters. Specifically, for two sands and a sandy clay loam, the saturated zone module predicts a high probability of achieving excellent nitrate removal. However, for an alternate case with lower denitrification values the amount of nitrate remaining in the aquifer can be significant.

3.2.6 HPS Corroboration and Limitations

The limitations of the saturated zone module and HPS solution have important implications for parameter values estimated via model calibration to field observations. Module corroboration shows that calibration of the denitrification parameter may result in an artificially low value due to agricultural nitrate concentrations or transverse advection due to water table mounding for points off the plume centerline. However, calibration utilizing observations approximately along the plume centerline may result in over estimation of the denitrification coefficient as the HPS solution tends to concentrate mass within this area. Other parameters estimated via calibration to field observations may also be over or under predicted for similar reasons.

The saturated zone module is a steady state model. To highlight the limitations of saturated zone module due to its steady state formulation, two numerical models (transient and steady state models) were also constructed and calibrated to observed field data. The comparison between the transient and steady numerical models and the limitation of each was used to infer the strength and weakness of steady state saturated zone module formulation. The transient model considered daily changes in the hydraulic gradient due to precipitation and ET. Because no data were available to account for daily fluctuations of nitrate mass flux to the aquifer, steady state contaminant loading was used. Also, boundary conditions were not capable of accounting for daily fluctuations in hydraulic head along model boundaries. These limitations in input data significantly limited the ability of the transient model to replicate observations. The groundwater flow portion of the model adequately replicated hydraulic head observations, though it was not capable of producing the observed variability within the observations. The contaminant transport portion of the model was unsuccessful in replicating the observed nitrate concentrations. The temporal variability in processes that control nitrate concentrations within the aquifer such as denitrification and mass flux as well as the limited input data for the model precluded any improvements.

Due to the poor results returned by the transient state model a steady state model was constructed for comparison to the saturated zone module. The steady state numerical model eliminated temporal variability and examined the average behavior over time of the aquifer and contaminant transport within the aquifer. While this model was primarily constructed for comparison to the saturated zone module to examine the significance of a three dimensional advection field, it revealed the limitations of transient state models. Transient state models require a significant amount of input data that may not be possible to obtain. Without this input data results from a transient model may be incorrect or difficult to interpret precluding the usefulness of such a model. Though it may seem desirable to evaluate an OWTS utilizing transient state models, results from the construction and calibration of the two numerical models demonstrates that this is not an effective approach. Capturing the average or long term behavior of the OWTS is assumed to be more useful and minimizes error. This analysis demonstrated that although transient models attempt to mimic the field conditions better than steady state models, their usefulness is significantly limited by the availability of data. Thus, for long term nitrate plumes within the aquifer, the steady state saturated zone module is a more useful tool.

While these limitations of the saturated zone module should be considered, they do not preclude the usefulness of module estimates. During saturated zone module corroboration it was concluded that denitrification was not as low as estimated by the saturated zone module via calibration. An independent laboratory evaluation of the denitrification potential of the same soils concluded that the denitrification rate was exceedingly low affirming the conclusion from corroboration (Farrell 2013; Farrell et al., 2014). Estimates of transverse horizontal dispersivity were likely less than reported from calibration of the aquifer model. However, if the user desires to estimate dispersivity with more accuracy a tracer test can be conducted. This illustrates that the saturated zone module is a versatile and powerful tool but that it does have limitations that should be recognized before using the model.

3.3 Multiple Spatial Inputs

This module calculates nitrogen mass flux [kg/yr] downstream at a specified distance from multiple sites. There are two separate modules (Multiple Sites I and II) incorporated into STUMOD-FL-HPS. The mass loading from each site is calculated to get the total mass loading at the down gradient point of interest.

For "Multiple Sites I", the mass flux at a point down gradient of the OWS is calculated in two steps. First, the nitrogen mass flux through the vadose zone to the water table is calculated using the vadose zone module, STUMOD-FL. Mass flux from STUMOD-FL is used as boundary input to the saturated zone HPS module.

For "Multiple Sites II", the module also calculates nitrogen mass flux [kg/yr] downstream at a specified distance. However, it assumes a known mass flux from the vadose zone to the water table for each site and no computations are made for the vadose zone. This module is applicable where estimates of mass loading to the water table are available and the user wants to use the saturated zone module only. Since "Multiple Site II" does not include a vadose zone run, it therefore takes a relatively shorter time.

There are two options for both the Multiple Site I and Multiple Site II approaches; the unique parameter set option and the lumped parameter set option. The unique parameter set option allows the user to specify individual site input parameters for both saturated and vadose zones. The mass loading from each site is calculated and the total mass flux is the sum of loading from each site. Thus, the model has to be executed several times to calculate the mass loading from each site requiring a longer run time, but allowing for variability in input parameters from the individual sites.

For the lumped parameter set option, users input parameters for each site, but parameter values for the sites are averaged together to calculate mass flux. In other words, averaged properties are used for the combined sites. This option takes a short time to run and is recommended for initial screening and when the sites are assumed to be very similar and the distance from each site to the down gradient point of interest are similar. If the site properties and distance to the point of interest are not similar, it should be noted that the results from the lumped approach would be very different compared to the unique parameter set option.

3.4 Performance Evaluation

There is always prediction uncertainty when using models to evaluate field conditions. This uncertainty may arise due to many reasons including variability and errors in the observational data, uncertainty in the model input parameters, and because the limitations of the model itself. No simulation model is an entirely true reflection of the physical process being modeled. Thus, when possible modeling results should be presented along with prediction uncertainty so model users can make more informed decisions. This concept was incorporated in STUMOD-FL where users can now generate cumulative frequency diagrams and make decisions based on probability rather than on point values generated by models from a single combination of input parameters. A sensitivity module has also been developed to help the user interpret which parameters the model output is most sensitive to.

3.4.1 Sensitivity Module

An automated sensitivity analysis module (Sensit) was added to STUMOD-FL. A sensitivity analysis indicates which input parameters are critical to and which parameters have less influence on the final model output. The sensitivity run can be used to compare the sensitivities of outputs to selected parameters (for a total of 8 parameters). The sensitivity module includes only a few primary operational parameters, such as hydraulic loading rate and effluent concentration, and other critical parameters such as nitrification and denitrification. The relative importance of these parameters in nitrogen removal is in the order of:

- hydraulic loading rate,
- porosity,
- effluent ammonium concentration,
- adsorption isotherm,
- nitrification rate,
- denitrification rate,
- soil temperature, and
- treatment depth (vadose zone thickness).

The approach used in the sensitivity analysis is that one input parameter is selected and its value is changed within a specified range while the other parameters are kept at their recommended value. The outputs distribution is then recorded. The process is repeated for all other input parameters producing output distributions for each input parameter. Output distributions are generated for each of the input parameters. The standard deviation of each output distribution was then compared and used as an indicator of the sensitivity of the output to the variability of the input parameter. For the purpose of comparison, the standard deviations are normalized by calculating the ratio of the standard deviation of each output distribution to the maximum standard deviation. Thus, the ratio varies from 0 to 1 and reflects the sensitivity of a parameter relative to the parameter with the highest sensitivity. The normalized values are sorted in descending order to rank the sensitivity.

3.4.2 Cumulative Frequency Diagram (CFD) Module

The CFD modules are intended to highlight uncertainties in the model estimates that may occur as a result of errors in the model input parameters. The CFD modules use Monte Carlo simulation to quantify the uncertainty of model outcomes. Monte Carlo simulations rely on random selection of input values for a model from a known parameter range producing a method for statistically quantifying the uncertainty of a model outcome.

For the vadose zone, the van Genuchten α and n, K_{sat}, Θ_r, and Θ_s and the nitrogen transformation parameters were all considered to have a log normal distribution. When the CFD module is executed, a model is executed numerous times with the input parameters selected randomly from ranges of expected values. The output of the model runs is then statistically analyzed and the probability of realizing any one particular outcome can be quantified, thus allowing the modeling results to be viewed in a risk-based framework (in a CFD) by displaying the cumulative uncertainty of a particular model output due to input data. The resulting model output can be viewed in a probabilistic framework allowing the user to determine which percentiles and outcomes are acceptable or unacceptable, or which outcomes represent "best," and "worst" cases. Rather than a single output, this approach gives the probability of realizing any one specific outcome, based on the cumulative uncertainty of all model input parameters. Two modules have been incorporated into STUMOD-FL-HPS: CFD I and CFD II.

The CFD I module generates a CFD for the percent of nitrogen at the water table using STUMOD-FL. Users may choose a 'soil type' and the number of runs. The results vary by soil type. The number of Monte Carlo simulations that are run is critical in establishing a valid cumulative probability plot. An insufficient number of runs will produce cumulative probability plots that are non-unique, meaning that if the same numbers of simulations are run again the shape of the subsequent cumulative probability plot will be slightly different. It was determined that that beyond 2000 simulations the plot did not change. For CFD I, the vadose zone flow parameters (α, K_{sat}, Θ_r, Θ_s, n and m), nitrification rate, denitrification rate, and soil temperature were varied. Outputs are generated for each combination of the inputs.

CFD II module generates a CFD for the percent of nitrogen at a down gradient distance using the HPS module. Users may choose a 'soil type' and the number of runs.

4 HOW TO USE THE TOOLS

Appropriate tool selection and use depends on the problem complexity, user expertise, technical resources, and treatment goals. Ideally, the simplest tools will be used first. Progressing through simple to more complex tools ultimately guides the user to the simplest tool that is appropriate, but discourages using a tool that is too simple for the decision at hand. In some cases, the tools may suggest additional information should be collected to increase the confidence in tool predicted nitrogen fate and transport. The importance of adequately describing key OWTS conditions in context of the problem or question at hand should not be over looked (e.g., soil properties, HLR, denitrification rates, etc.). Interpretation of tool outputs must be done in context of the current knowledge of the site conditions, scientific principles, and treatment and performance goals. It is only in this manner that the user can make better-informed decisions that account for the uncertainty in the OWTS nitrogen fate and transport processes.

4.1 Visual Tools

The simplest tools developed are visual tools including look-up tables and HYDRUS-2D simulation outputs. Two types of look-up tables are provided: 1) summary information from the literature, and 2) summary information from HYDRUS-2D model simulations.

4.1.1 Summary Data for Parameter Selection

Visual tools provide an indication nitrogen fate and transport for specific technical assumptions, site conditions, and OWTS operating factors. The first look-up tables summarize model input parameters based on evaluation of literature values. When sufficient data are available, CFD diagrams are provided to enable better understanding of the assimilated data (e.g., see Section 3.2.3 on saturated denitrification rates). The cumulative frequency as a percentage is presented on the y-axis and the reported values are presented on the x-axis. The CFD enables the user to select a value from a range of actual reported data that incorporates an acceptable uncertainty for a specific condition. In most cases data is not sufficient to allow further analysis specific to Florida conditions (e.g., ammonification) and McCray et al., 2010 should be referenced for greater understanding of the data assumptions and limitations within the vadose zone module (STUMOD-FL) default parameters.

However, important information that affects performance, such as STE nitrogen concentrations (see Section 3.1.1) and soil properties (see Appendix A) could be tailored to Florida. Soil properties were evaluated based on data in the Florida Soil Characterization Data Retrieval System (University of Florida, 2007). Data records were sorted by soil textural classification and then screened for complete data sets (incomplete data sets were removed from further analysis) and data records applicable to depths of less than 5ft below ground surface.

Due to the prevalence of sandy soil textures in Florida, and in context of the finding that relatively few soils series comprise the majority of the land area, a sand soil series was included for further evaluation if the series was ranked in the top 30 of any of three following criteria: 1) most frequently permitted soil series (based on number of recent permits issued), 2) largest areal extent based on total land area (acreage) in Florida, or 3) largest areal extent (again based on acreage) within all sand series. All sand textures (sand, fine sand, very fine sand, etc.) were included in the analysis. Excluded from the analysis were the Urban series. This approach resulted in analyses of 1,799 complete data records representing 40 individual sand series.

To determine model parameters for sandy clay loam, an individual data record was included for evaluation based on three criteria: 1) the Florida Soil Characterization Data Retrieval System listed the textural classification as "sandy clay loam", 2) the series was included in the top 60 frequently permitted soil series, *and* 3) the series was included within the top 60 largest areal extent based on total land area in Florida. This ensured that the data evaluated was representative of a sandy clay loam even though the series and/or shallow depths might have a higher sand fraction (e.g., Orangeburg, Dothan, etc.). This approach resulted in analyses of 122 complete data records representing 31 individual soil series.

Relative to the sand textures, less data was available for other soil textures (loamy sand, sandy loam, loam, silt loam, silt, silty clay loam, sandy clay, clay loam, and clay) in the Florida Soil Characterization Data Retrieval System. For these remaining soil textures, a data record was included for evaluation based on the textural classification listed in the Florida Soil Characterization Data Retrieval System and soil depths <5 ft below the ground surface. For silts, only 11 data records were in the Florida Soil Characterization Data Retrieval System and of these 11 data records, only two were complete data records in the top 5ft of soil. Rather than omit silt textures from STUMOD-FL, the Data Retrieval System was sorted by the % silt and complete records with silt fractions >40% were retained for further analysis. This subset, was further sorted by the silt fraction to identify data records for silt (>87% silt and <20% sand), silt loam (73 – 87% silt and < 50% sand), silty clay loam (>60% silt and >25% clay), and silty clay (> 40% silt and >40% clay). There were no records that qualified as a silty clay.

Additional detail on determining soil parameters is presented in the FOSNRS Tasks D.7 and D.8 reports. Look-up tables summarizing this evaluation and the resulting default parameters by soil series are presented in Appendix A. In addition, a worksheet listing the most common Florida soils and the associated parameters is included within STUMOD-FL-HPS. These look-up tables should be considered starting points for cases were addition information might not be available. The user can select any data set (e.g., different depths, different soil series, etc.) from the Florida Soil Characterization Data Retrieval System as appropriate or determine parameters based on soil data obtained in the field.

4.1.2 Summary Data for HYDRUS-2D Simulations

Look-up table information, in electronic format, was provided summarizing the HYDRUS-2D simulations (see FOSNRS Task D.7 file "HYDRUS Output Summary.xlsx"). The values reported related to nitrogen concentrations and mass fluxes are based on the assumptions incorporated in the simulations, or numerical model limitations. Information provided by these simple tools is based on data generated by a numerical model that can incorporate complex treatment and operating conditions. More detailed description of the assumptions used in HYDRUS-2D scenario analysis is described in the Task D.7 while a summary is provided below.

HYDRUS-2D (Šimůnek et al., 1999) was used to simulate steady-state unsaturated transport of nitrogen species in saturated soils for the purpose of demonstrating the effect of design and operating conditions on STU performance. For the simulations, a modified version of HYDRUS-2D was used that accounts for the effect of aeration via soil moisture content and temperature on treatment allowing assessment of nitrogen transformation under a variety of OWTS loading conditions.

HYDRUS-2D simulations were run for selected conditions representative of Florida to illustrate the subsurface affects that can be attributed to changes in operational or environmental conditions. Scenarios included variations in distribution configurations, soil textures, effluent quality, subsurface heterogeneity and water table depths (Table 4.1). All simulations were run to steady state conditions as determined by no change in the predicted water profile or nitrogen concentrations with additional simulation time. A constant loading rate was used with effluent applied to the infiltrative surface of a homogeneous subsoil layer overlain by a lower permeability biozone. Limited additional simulations considered a variety of layered soils to account for subsurface vertical heterogeneity.

Table 4.1: Key Operating Conditions Varied during HYDRUS-2D Simulations

Condition	Variations Simulated
Distribution Configuration	Trenches, equal effluent distribution to each trench; Trenches, unequal effluent distribution to each trench; Bed, equal effluent distribution to each bed; or Bed, unequal effluent distribution to each bed.
Soil Texture	sandy clay loam; less permeable sand; or more permeable sand.
Soil Profile	homogenous; or layered
Effluent Nitrogen Composition	typical STE; or nitrified effluent.
Depth to Water Table	1 ft below the infiltrative surface; 2 ft below the infiltrative surface; 6 ft below the infiltrative surface; or free drainage (deep water table).

Simulations were run with an assumption of free boundary conditions (i.e., a deep water table) or with a constant head boundary condition at 1, 2, and 6 ft below the infiltrative surface. Two general effluent qualities were considered: typical STE and nitrified effluent. Typical STE was represented by 60 mg-N/L as ammonium nitrogen with no nitrate nitrogen. The nitrified effluent was assumed to be partially treated having 15 mg-N/L as ammonium nitrogen and 15 mg-N/L as nitrate nitrogen based on input provided by FDOH. For both effluent qualities, sufficient carbon required for both nitrification and denitrification reactions were assumed. It was also assumed that sufficient alkalinity was present and that the pH and temperature were within a range where sufficient nitrification and denitrification occurs.

Several additional parameters are required by HYDRUS-2D to simulate nitrogen transport and transformation (e.g., nitrogen transformation rate constants, ammonium sorption constants, etc.) and are described in the Task D.7 report with additional detail provided in McCray et al., 2010. In general, parameter selection was based on statistical distributions of data obtained in the literature. From these data, mean values with standard deviations or median values with quartiles, and/or the cumulative frequency of parameter values were calculated previously (McCray et al., 2010). Scarcity of data sometimes precluded this approach (e.g., for ammonium sorption constants).

Also provided in the FOSNRS Task D.7 report are numerical model simulation outputs of different OWTS scenarios to visually demonstrate both the impacts of different scenarios on subsurface water content, ammonium-nitrogen concentrations, and nitrate-nitrogen concentrations as well as the usefulness of such a numerical model.

The D.7 look-up tables and graphical displays are simple tools developed using steady state HYDRUS-2D simulations. These simple tools are intended to provide insights into expected OWTS behaviors as a result of changes in site-specific and operating conditions. A steady state model does not incorporate many of the complexities associated with OWTS treatment processes, nor capture diurnal variations, short term influences, or system perturbations. However, a steady state is still appropriate for the development of the simple tools since the main objective in this case is to get an understanding of the relative differences in responses (concentration at the water table or mass loading) as a result of change in site-specific conditions (e.g., soil texture) or operating conditions (e.g., configurations or effluent concentrations).

Because the illustrations for representative OWTS conditions are limited, the user must decide how their OWTS system fits within the limited treatment estimations displayed by the visual tools. Corroboration with field data at the USF Lysimeter Station and the FOSNRS GCREC soil and groundwater test sites showed that including precipitation resulted in lower model estimates of nitrogen flux because of a dilution effect. The simple tools developed based on steady state produced a more conservative estimate (less nitrogen removal or a higher nitrogen flux) representative of what would occur during an extended dry period each year and are desirable from design perspective.

4.2 STUMOD-FL-HPS

STUMOD-FL-HPS, is a combined aquifer-complex soil model where a vadose zone module, STUMOD-FL, is coupled with the HPS aquifer module providing the user with the ability to seamlessly evaluate contaminant transport through the vadose zone and aquifer underlying an OWTS. The model has been implemented as an Excel Visual Basic Application (Excel VBA) with multiple modules (Figure 4.1) to allow easy implementation by a wide range of users while also providing flexibility to evaluate a wide range of scenarios:

- vadose zone fate and transport (STUMOD-FL),
- saturated zone fate and transport (HPS),
- combined vadose and saturated zone fate and transport (STUMOD-FL-HPS),
- multiple OWTS inputs (Multiple Sites I and Multiple Sites II),
    - similar parameters
    - unique or varying parameters
- sensitivity analysis (Sensit), and
- uncertainty analysis.
    - vadose zone (CFD I)
    - saturated zone (CFD II)

STUMOD-FL-HPS is compatible with Microsoft Excel 2011 versions and higher. Macros must be enabled. Certain functions (e.g., drop down menus) are not compatible with Apple Excel versions.

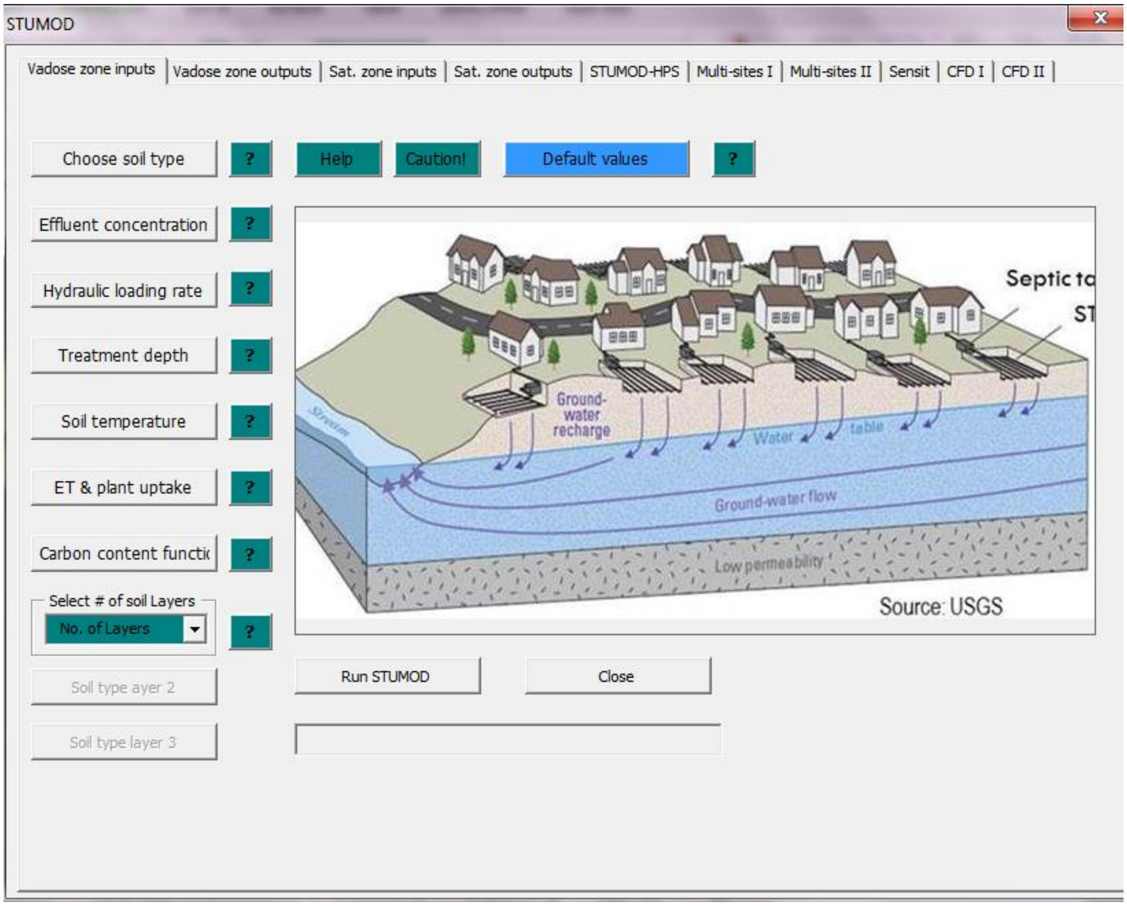

Figure 4.1: STUMOD-FL-HPS graphical user interface showing module tabs.

The following provides guidance on the general use of the STUMOD-FL-HPS modules. First, guidance on the use of the vadose zone module (STUMOD-FL) is presented. This module is used to calculate concentration and mass loading in the unsaturated zone at the water table or a user specified treatment depth. The inputs to STUMOD-FL include soil hydraulic parameters, loading rate, effluent concentration and nutrient transformation parameters. The model also accounts for the effect of oxygen via soil moisture content, soil temperature, carbon content and plant uptake. The effects of ET, plant nutrient uptake, and multiple soil layers have been incorporated. STUMOD-FL has built in default parameter but allows the user to change parameters and can be calibrated to site-specific data.

The saturated zone HPS module is used to calculate mass loading down gradient of a soil treatment unit. The inputs to HPS include operational, aquifer, and contaminant properties. As in STUMOD-FL, default parameters are built in, but the module allows users to change the parameters and can be calibrated to site-specific data.

The multiple sites modules are used to calculate mass loading down gradient (at a well or water body) of soil treatment units from multiple sites. These modules are good screening level tools for larger developments and provide several options within the modules to allow flexibility in the approach based on available data and the question of interest.

The sensitivity module is used to calculate parameter relative sensitivity in the vadose zone. A sensitivity analysis indicates which input parameters are critical to and which parameters have less influence on the final model output. This approach is important to helping the user interpret the STUMOD-FL outputs.

The CFD modules generate CFDs based on user input ranges of specific parameters of either concentrations the water table (CFD I) or of mass loading down gradient of a soil treatment unit (CFD II).

4.2.1 How to Use the Vadose Zone Module - STUMOD-FL

The inputs to the vadose zone module include soil type, effluent concentration, hydraulic loading rate, treatment depth, temperature, ET & plant uptake, and carbon content function listed on the left side of the graphical user interface (GUI) (Figure 4.2). Users can click on each button to populate various vadose zone model parameters. After clicking on each button, an input form appears. Default parameters are provided in each case; however, users can modify inputs different from the default value.

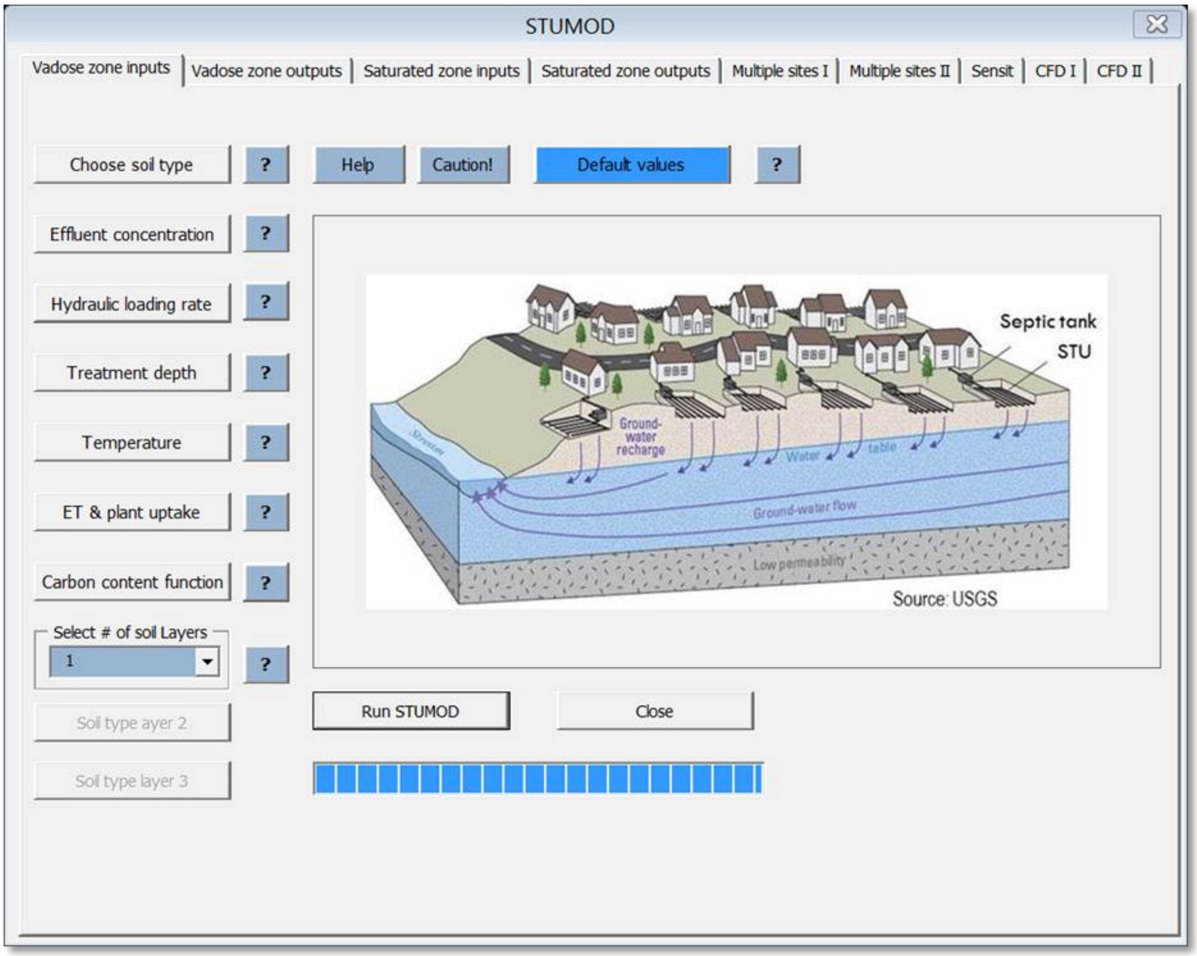

Figure 4.2: Main page of the STUMOD-FL graphical user interface.

The tool stores all the input data used in the current run. Users do not need to re-enter the data previously already entered during the session (note, all default values will be returned with the model is closed). Users need to enter the data only for those inputs they want to change. Values used in the current run are also stored in the 'Input Summary' worksheet.

Users may want to restore all the inputs to some default values and start with a new set of data. By clicking on the 'Default values' button on the top right, all input values will be reset back to defaults. When opening STUMOD-FL, the default soil type is more permeable sand, the effluent concentration is 60 mg-N/L NH_4, the hydraulic loading is 2 cm/d, and the water table is at 60 cm. There is no plant uptake or ET as a default.

4.2.1.1 Soil Type and Parameters

Users can choose between 13 different soil types (Figure 4.3). When a soil type is selected, hydraulic parameters, nitrification, denitrification, sorption rates and other parameters listed in Figure 4.3 are automatically populated. Under the 'Parameter input options' (second column), users may select either 'Default values' or 'User Inputs' options from the drop down menu. To make any changes to the input default values, the 'User Inputs' option must be selected then the soil hydraulic properties, reaction and sorption rates or other parameters can be updated. After choosing the soil type or modifying the input data, click on 'update values' inputs button at the bottom to send the inputs to the input table.

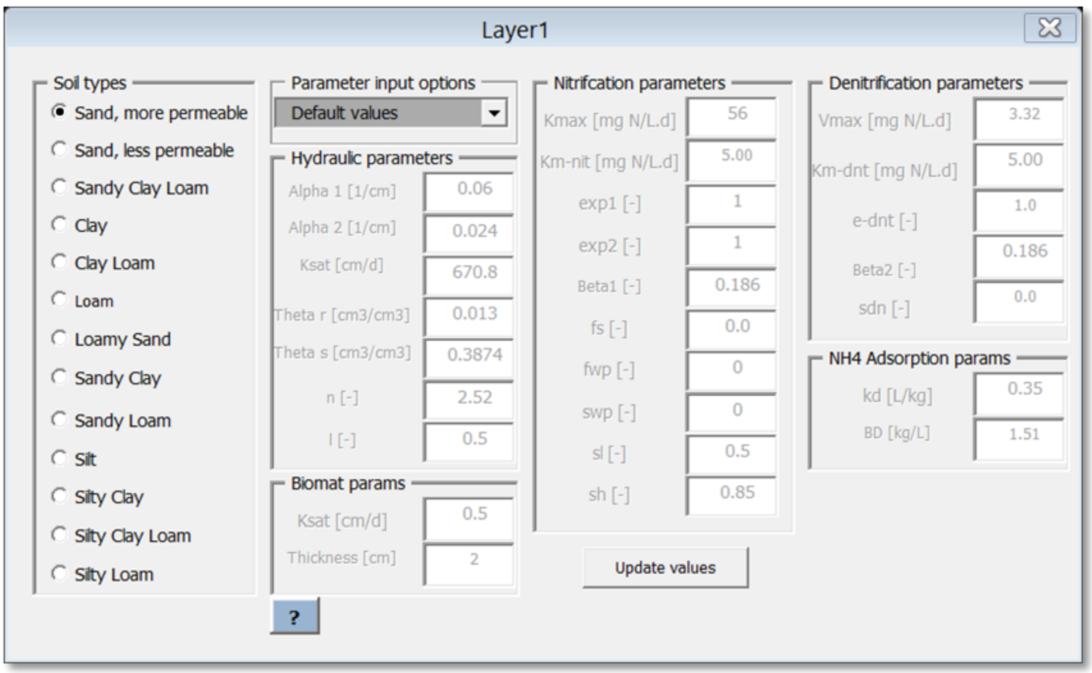

Figure 4.3: STUMOD-FL GUI for soil parameters.

4.2.1.2 Effluent Concentration

To adjust the input effluent concentration, click on the 'Effluent concentration' button from the main page (Figure 4.2). The input form below (Figure 4.4) will be displayed. Default values for septic tank effluent (STE) ammonium and nitrate concentration are provided. Typical STE was assumed to be 60 mg-N/L as ammonium-nitrogen and little or no nitrate-nitrogen. Users can input a wide range of new values including nitrified effluent represented by low ammonium and higher nitrate concentrations.

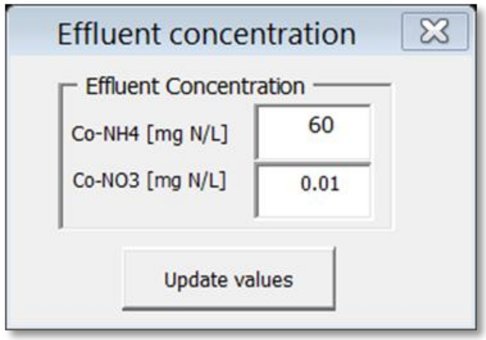

Figure 4.4: STUMOD-FL GUI for effluent concentration.

Click 'update values' button if any changes are made to effluent concentration inputs.

4.2.1.3 Treatment Depth

The default value for treatment depth is a water table depth (WTD) at 2 ft or 60 cm below the infiltrative surface. However, users can change the water table depth or treatment depth using the options listed under the 'Treatment depth' form (Figure 4.5) by clicking on 'Treatment depth' option from the main page (Figure 4.2). Three options are provided under the 'Water Table Options' drop down menu in the input form (Figure 4.5).

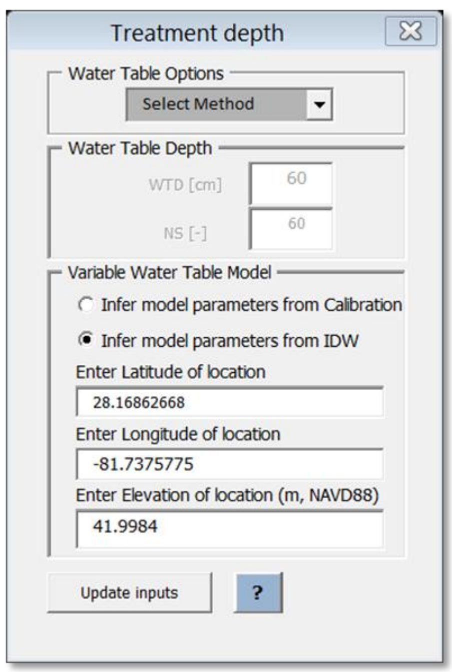

Figure 4.5: STUMOD-FL GUI for treatment depth inputs.

The first option is 'user input WTD'. This is the easiest option and is used when the water table depth is known or can be closely approximated. For this option, the WTD is input as centimeters below the infiltrative surface. STUMOD-FL calculates concentration reaching this user defined WTD. In this case, the soil moisture content is affected by capillary rise. Nitrogen removal rates are higher at the capillary zone due to relatively higher moisture content as defined by the soil moisture response function for denitrification (assuming carbon content is not limiting, see Section 4.2.1.6). 'NS' refers to the number of segments. The user input WTD is divided into segments for computational purposes. The default number of segments is set to 60. Increasing the number of segments provides additional computational resolution, but requires more time to run.

When the second option, 'calculated WTD', is selected, the water table depth is calculated by the model. An analytical model is incorporated for water table fluctuations in response to precipitation in this option. Parameters for the water table fluctuation can be inferred via calibration using known historical precipitation (when 'infer water table depth calibration' is selected), or known historical water table data, or from an inverse distance weighting approach based on topographic data (when 'infer water table depth from IDW' is selected). This is a good option when the water table is expected to be relatively deep, but the 'user input WTD' option first described is generally the recommended option.

The third option, 'deep WT', is a deep water table where the groundwater is assumed to be deep resulting in free drainage conditions. Thus, there is no effect of soil moisture due to capillary. In this option, the value input is used as an arbitrary treatment depth specified by the user, not a water table depth. The input for NS can be varied, but generally should remain at 60.

Click 'update inputs' button if any changes are made to treatment depth inputs.

4.2.1.4. Soil Temperature

Reaction rates in STUMOD-FL are adjusted for temperature. The adjustment factor varies between 0 and 1, with an adjustment factor of 1 at optimum temperature. The optimum temperature in STUMOD is 25 °C. The adjustment factor is <1 for temperatures either lower or higher than the optimum temperature. The adjustment factor is calculated by the model based on the user input temperature (Figure 4.6). Guidance for selecting appropriate temperatures can be found at http://www.wcc.nrcs.usda.gov/scan/. The options Topt1 and Topt2 are optimum temperatures for nitrification and denitrification respectively, and should not be altered unless additional information is available.

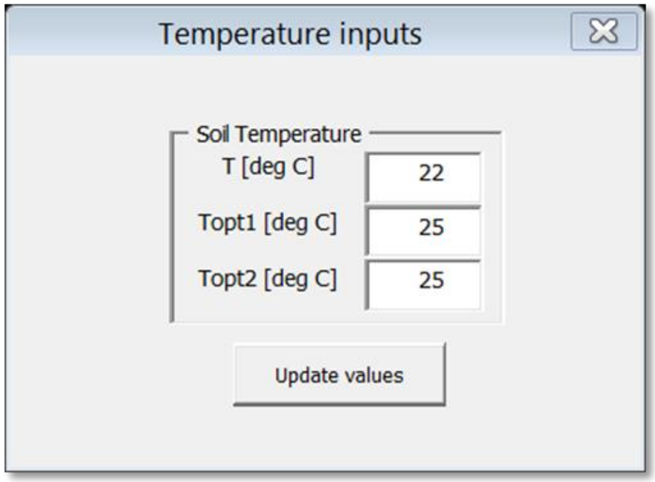

Figure 4.6: STUMOD-FL GUI for soil temperature inputs.

Click 'update values' button if any changes are made to temperature inputs.

4.2.1.5. Evapotranspiration (ET) and Plant Uptake

Plant water uptake (ET) or in STUMOD is based on potential evapotranspiration (PET) adjusted for the effect of soil moisture content & root distribution. Plant nutrient uptake depends on plant water uptake & concentration of ammonium and nitrate in soil solution calculated by STUMOD. On the main page (Figure 4.2), click on 'ET & plant uptake' button and the associated input form shown in Figure 4.7 will come up. Choose 'No' under the 'Water & nutrient uptake' dropdown menu to ignore plant uptake if there is no vegetation on the site. 'No' plant uptake is the default. If plant uptake is to be included select 'Yes' and the associated ET parameters will be unlocked for user changes.

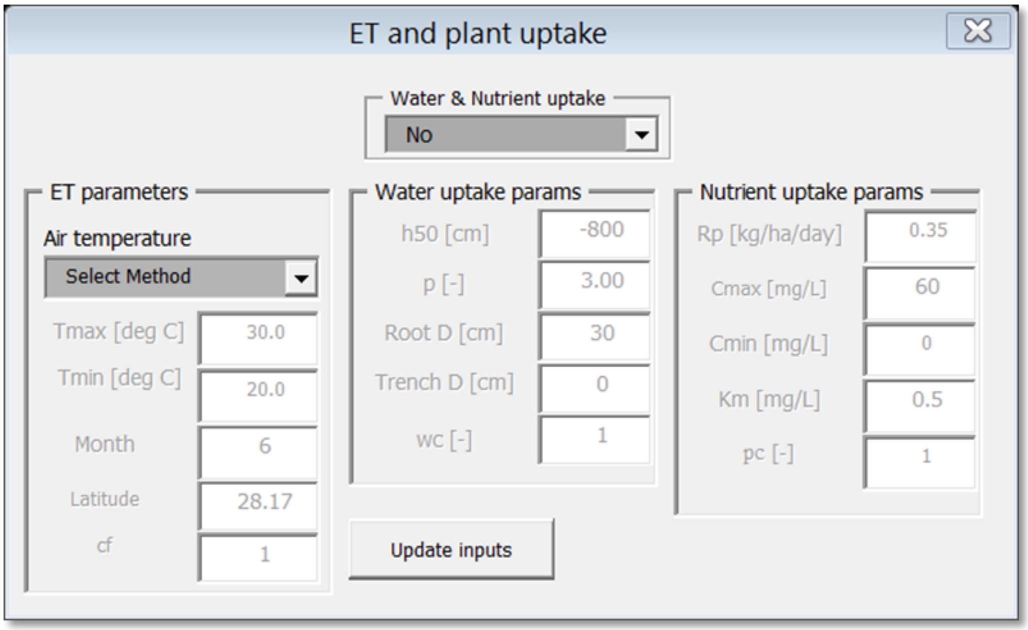

Figure 4.7: STUMOD-FL GUI for ET and plant uptake inputs.

The ET parameters in the left column (maximum and minimum temperature, month, and latitude) are parameters used to calculate PET using Hargreaves Method. The month number varies from 1 to 12, starting from January, January =1, February=2, etc. Latitude should be representative of the site location. C_f is a calibration parameter to adjust PET estimates from Hargreaves equation. The actual ET or plant uptake is calculated from PET and then adjusted for soil moisture status and root distribution. The adjustment factors for both soil moisture and root distribution vary from 0 to 1.

The center column for 'Water uptake params' lists parameters needed for the soil moisture adjustment factor (see equation 3-2, Section 3.1.5 above, and the Task D.8 report for additional detail). STUMOD calculates suction with depth, thus, suction outputs from STUMOD are used as input to calculate actual ET. The two parameters in equation 3-2, h_{50} and p_1, are set to -800 and 3 respectively. 'Root D' is the root depth can be changed by the user and is in centimeters from the land surface. 'Trench D' is the depth of the infiltrative surface below the land surface, again in centimeters. Plant roots must extend below the infiltrative surface for either water uptake or plant nutrient uptake to occur. w_c is a calibration parameter with a value between 0 and 1 to adjust for the root density with depth. The value is set to 1. A value of 1 implies no adjustment. A value less than 1 can be used to increase the water uptake (note that w_c is a divisor, not a multiplier).

The right column for 'Nutrient uptake params' (Figure 4.7) lists the parameters needed for both passive and active nutrient uptake assuming the roots extend below the infiltrative surface (see Task D.8 for additional detail). R_p is the potential nutrient demand, C_{max} is the maximum nutrient concentration that can be taken up by plant roots, C_{min} is the minimum concentration needed to initiate nutrient uptake. P_c and k_m are calibration parameters. The passive nutrient uptake term can be turned off by selecting c_{max} equal to zero. Active nutrient uptake can be eliminated by specifying a very large c_{min} value. These parameter values are assumed to be both nutrient and plant specific. To ignore plant uptake, the user can set R_p = 0.

Click 'update inputs' button if any changes are made to any ET or plant uptake inputs.

4.2.1.6. Carbon content function

STUMOD-FL considers the effect of carbon availability on denitrification. Two sources of carbon are considered, carbon content from STE and naturally occurring in the soil. Carbon function inputs are shown in Figure 4.8. The user generally enters only the BOD5 concentration known or estimated in the STE, 'C_o STE', although other parameters can be changed. The soil carbon is automatically added based on the soil type selected.

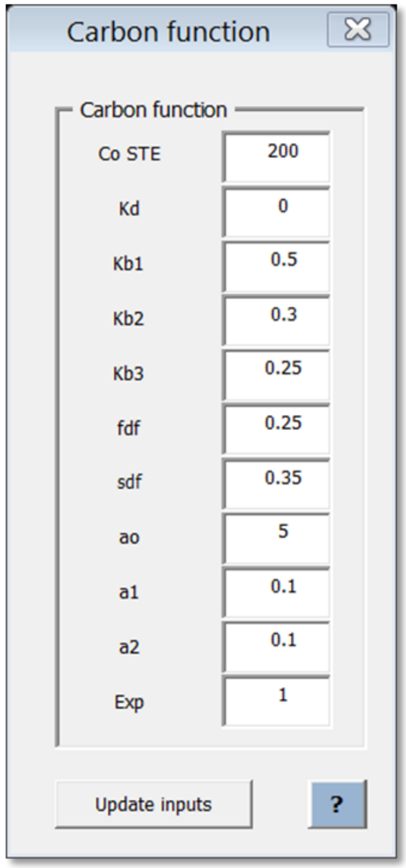

Figure 4.8: STUMOD-FL GUI for carbon content inputs.

For the carbon in STE, STUMOD assumes a ratio of 8:1 for BOD:carbon based on the user input STE BOD. Of this carbon in STE, it is assumed to have fractions of easily biodegradable carbon, moderately biodegradable carbon, and slowly degradable carbon represented by degradation rates of K_{b1}, K_{b2}, and K_{b3}, respectively. The default values for K_{b1}, K_{b2} and K_{b3} are 0.5, 0.3 and 0.25/day. The relative fraction of each type of biodegradable STE carbon can be modified with 'fdf' as the fraction of fast degradable portion, default value of 0.25, and 'sdf' as the slow degrading fraction, default value of 0.35. The remaining fraction is calculated by the model as the moderately biodegradable fraction. K_d is the sorption rate set to zero and α_1, α_2, and α_3 are calibration parameters for K_{b1}, K_{b2} and K_{b3}.

Carbon availability with depth is assumed to change with rate of denitrification. Thus, K_{b1}, K_{b2} and K_{b3} are further adjusted for soil moisture and temperature (see the Task D.10 report). This dependency on soil moisture content coupled with differences in travel time results in a changing carbon profile with depth allowing for carbon from STE to percolated deeper into the soil profile in sandy soils compared to clayey soils. 'Exp' is an exponent relating the depth distribution of carbon content with soil moisture or consequent denitrification rates.

Click 'update inputs' button if any changes are made to any carbon inputs.

4.2.1.7 Selecting Layers

The default in STUMOD-FL is a single homogenous layer. Additional layers can be added after defining the input parameters listed in the main page (Figure 4.2) for the homogenous layer (see Section 4.2.1.1). Select the total number of layers of interest from the drop down menu 'Select # of Layers' at the lower left of the main page. The model will prompt the user to select the 'Soil type layer 2' button to input soil parameters (Figure 4.9). After entering the input, click the 'update inputs' button. If 3 layers are selected (maximum number of layers in STUMOD-FL), then click on either the 'Go to layer 3' button on the layer 2 input page or return to the STUMOD-FL main page and select the 'Soil type layer 3' button. Again, click on 'update values' after entering soil parameters for layer 3.

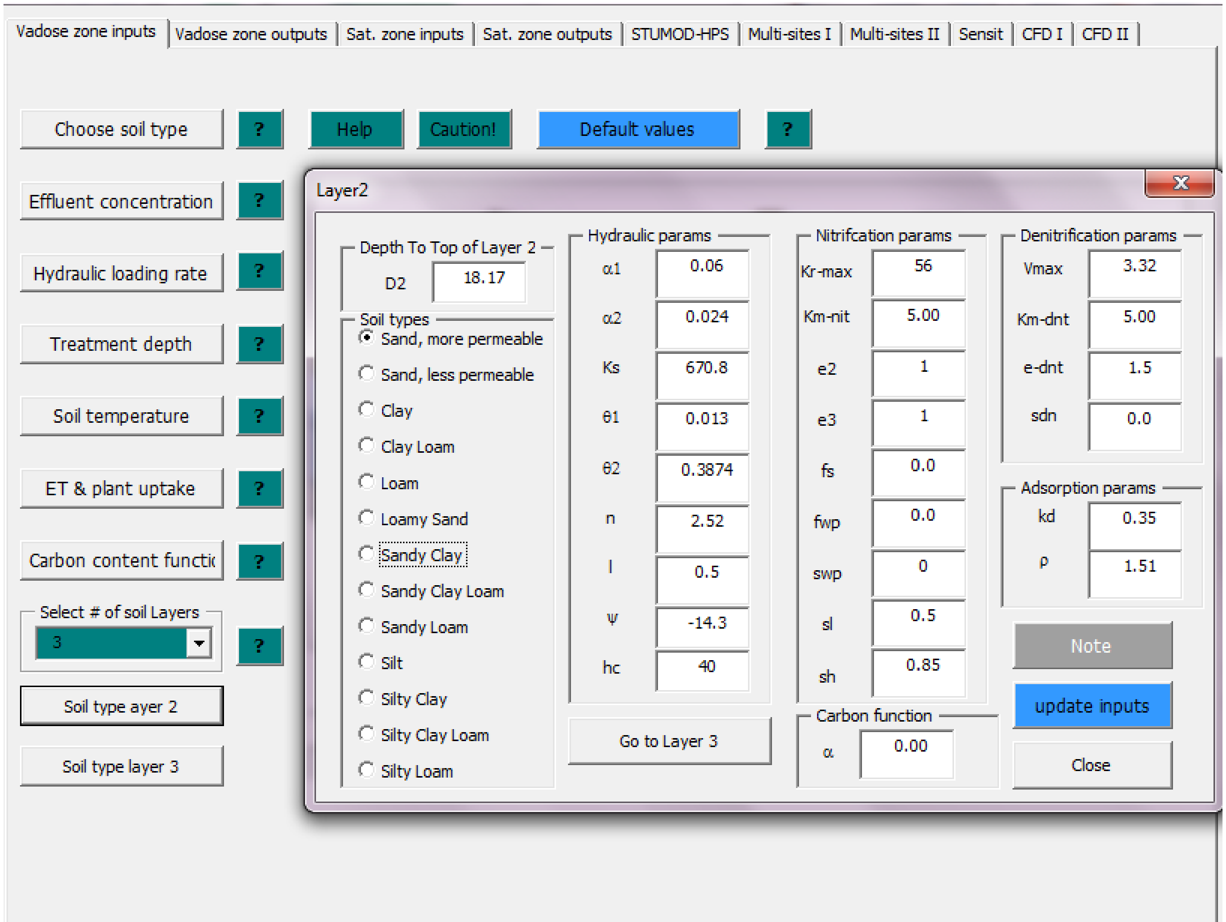

Figure 4.9: STUMOD-FL GUI showing multiple soil layer inputs.

4.2.1.8 Running STUMOD-FL

After defining the input parameters listed in the main page (Figure 4.2), Select the 'Run STUMOD' button to execute the module. To view the outputs, go to the 'Vadose Zone Outputs' tab. The vadose zone (unsaturated zone) outputs are shown in Figure 4.10.

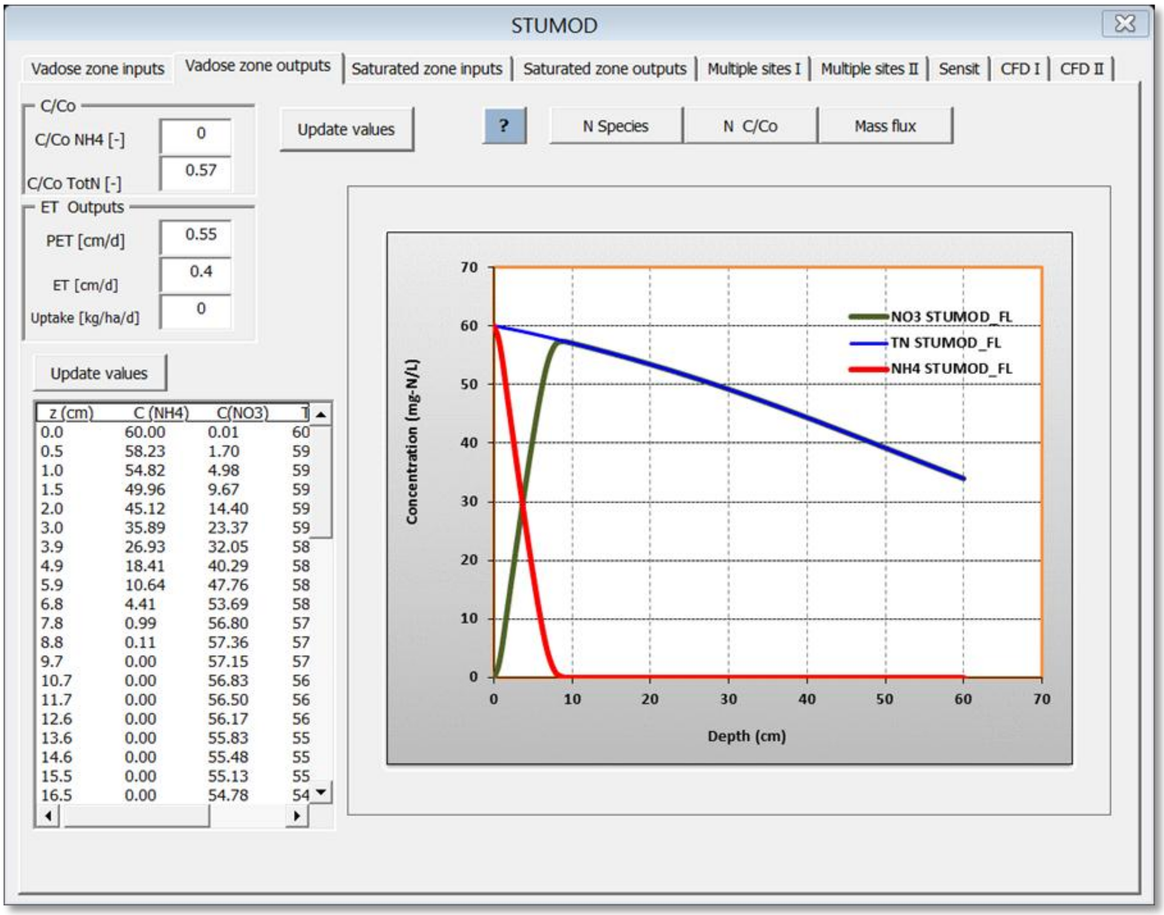

Figure 4.10: STUMOD-FL GUI showing vadose zone outputs.

The outputs under 'C/Co' are the fraction of ammonium (NH4-N) and the fraction of total nitrogen (TN) remaining at the water table (or user specified treatment depth). The 'ET ouputs' are the calcuated PET, actual ET (cm/d), and plant nutrient uptake (kg/ha/day) values.

A graphical output for ammonium (NH_4-N), nitrate (NO_3-N) and total nitrogen (TN) can be displayed by clicking on the 'N Species' button. Clicking on the 'N C/Co' button will display a graph for the fraction of total nitrogen remaining with depth. Clicking on the 'Mass flux' button will display the estimated mass flux with depth.

Tabular outputs for NH_4-N, NO_3-N and TN with depth can also be displayed by clicking on the 'Update values' button on the left above the table. Tabular outputs for NH_4-N, NO_3-N and TN can also be obtained from 'VZ_N_out' worksheet, columns AJ to AO, for export to external software.

By returning to the main page (Figure 4.2) the user can change any or all parameters by following the above steps in Section 4.2.1 and again clicking on the 'Run STUMOD' button. Upon closing the model, all user defined inputs will be lost and default values will be returned.

4.2.2 How to use the Saturated Zone Module - HPS

The saturated zone module, HPS, uses an analytical contaminant transport equation that is ideally suited for an OWTS and simplifies user input. The saturated zone module, HPS, can be run independently or coupled with STUMOD providing the ability to seamlessly evaluate contaminant transport through the vadose and saturated zones. The saturated zone module Graphical User Interface (GUI) facilitates user interaction making the model easy-to-use.

Like the STUMOD-FL input main page, the HPS input main page, 'Sat. zone inputs', has a list of major inputs including OWS dimensions, aquifer properties, contaminant properties, and groundwater velocity (Figure 4.11). In addition, output options allow the user to choose how the results are to be viewed. Clicking any of the input buttons on the left will display an input table allowing users to populate saturated zone model parameters. Default parameters are provided in each case; however, users can modify inputs if different from the default value.

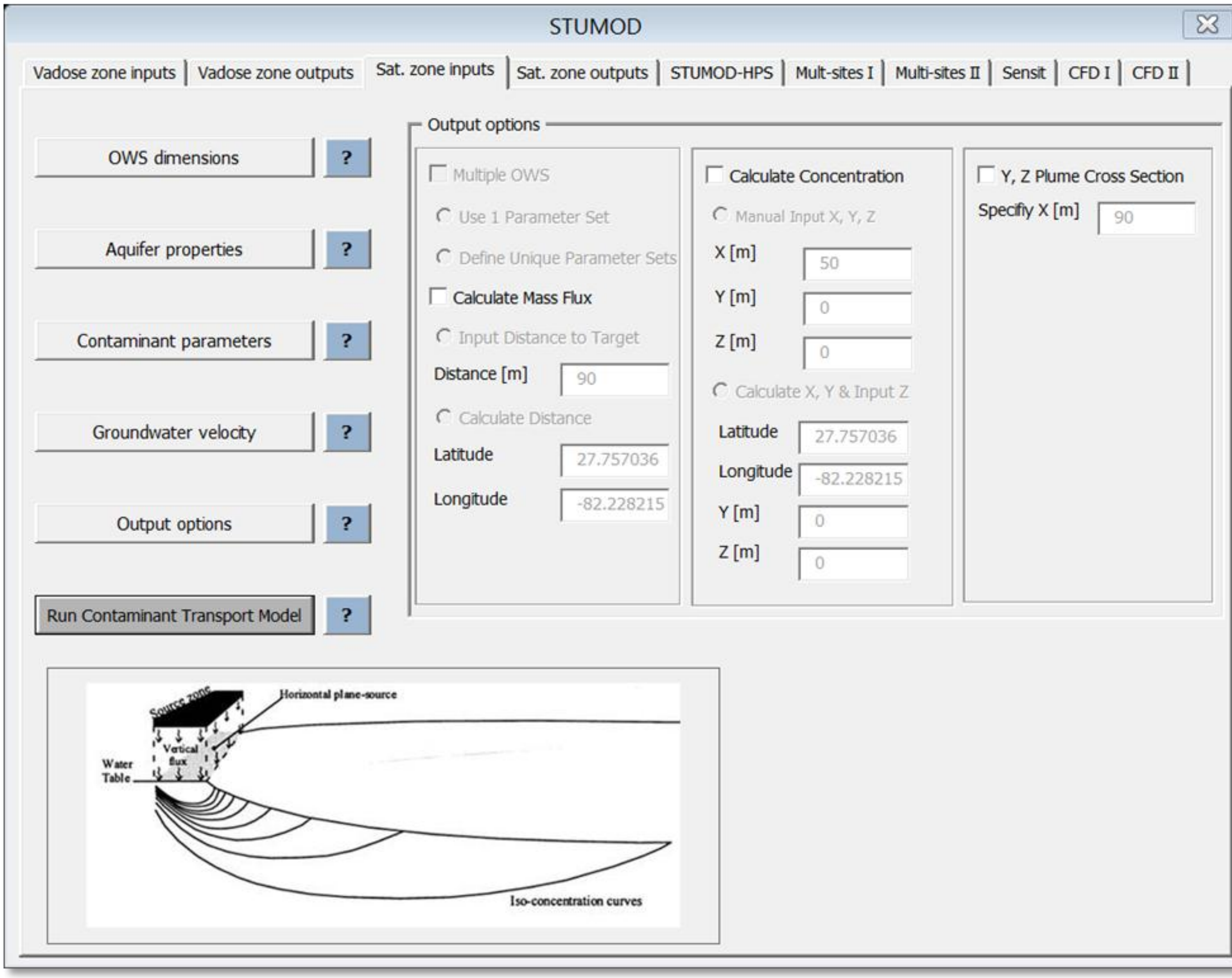

Figure 4.11: Main page of the saturated zone module, HPS, graphical user interface.

4.2.2.1 OWS Dimensions

First the user must choose either a 'Bed' or 'Trench' configuration. When a 'Bed; configuration is selected, the user must enter a width, length, and hydraulic loading rate, 'Rate'. When a 'Trench' configuration is selected, users must enter the number of trenches, trench spacing, trench width, and trench length. The loading rate is populated automatically from STUMOD-FL outputs.

For both 'Bed' and 'Trench' selections, the location of the OWTS (latitude and longitude of the center of the OWS) is used only if the location of a down gradient distance is specified using latitude and longitude listed under the 'outputs options'. The location inputs are not used if users choose a down gradient distance option instead of lat-long inputs.

At the bottom of the 'OWS Dimensions' input table (Figure 4.12), users store the changes made by clicking on the 'Store values' button. If the user would like to retrieve the previously input parameters, they can click on the 'Previous values' button. Either button must be selected to save the input changes.

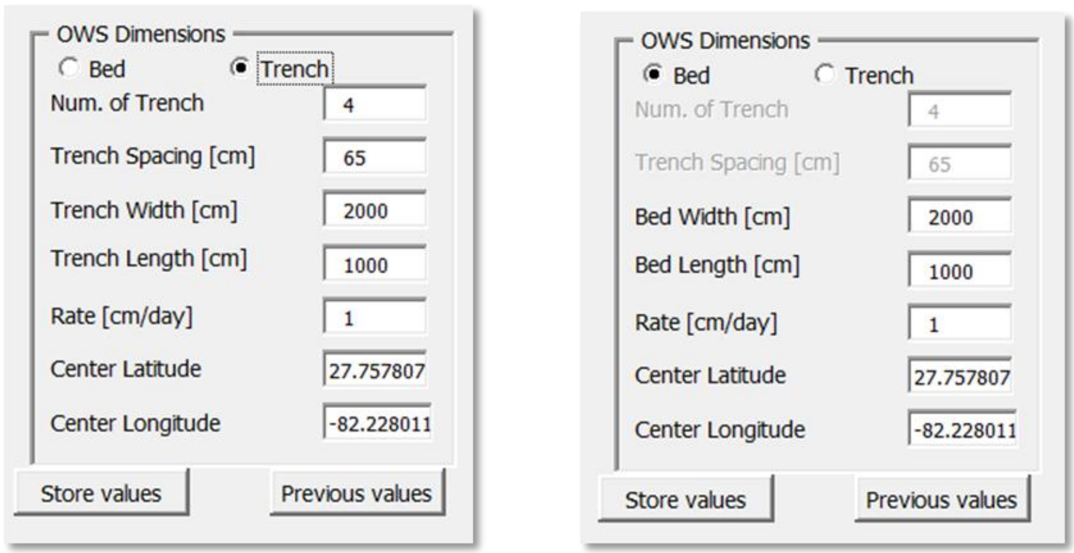

Figure 4.12: HPS GUI showing OWS inputs.

4.2.2.2. Aquifer Properties

Inputs specific to aquifer properties include porosity, X-dispersivity, Y-dispersivity, Z-dispersivity, saturated hydraulic conductivity and aquifer thickness (Figure 4.13). Default values for porosity and saturated hydraulic conductivity are imported from STUMOD-FL but users can modify the values if they are expected to be different for the saturated zone. Parameter values for X-dispersivity, Y-dispersivity, and Z-dispersivity can either be input by the user or calculated by the model. If the user would like to use model-calculated values, check the 'Estimate Dispersivity' box at the bottom of the menu and dispersivity values are estimated based on flow length. The aquifer thickness is the depth from the average water table elevation to the top of a confining layer if present. If a confining layer is not present, large values such as 100 m should be used.

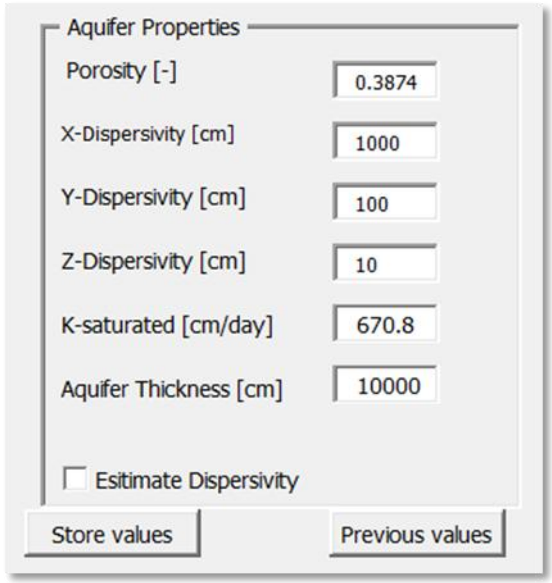

Figure 4.13: HPS GUI showing aquifer property inputs.

After changes are made, click on the 'Store values' button to save the inputs. Stored values can be used later by clicking 'Previous values' button.

4.2.2.3. Contaminant Parameters

The contaminant parameters utilized by HPS include the retardation factor, decay rate, and concentration (Figure 4.14). The nitrate concentration estimated by the STUMOD-FL module at the water table will be automatically populated in the 'Concentration' field from the previous STUMOD-FL run. In this case, the user would have selected 'user input WTD' in STUMOD-FL (Section 4.2.1.3, STUMOD-FL Treatment Depth inputs). However, input concentrations can be modified if HPS is run independently or the concentration at the water table is known or can be estimated. Concentration is as nitrate-nitrogen. The 'Retardation factor' allows flexibility of modeling the transport of other contaminants, such as ammonium. The default retardation factor of 1 result in no retardation and nitrate is transported at the average seepage velocity. The 'Decay Rate' is the denitrification rate (in 1/d). Default values are provided, but users can modify these inputs.

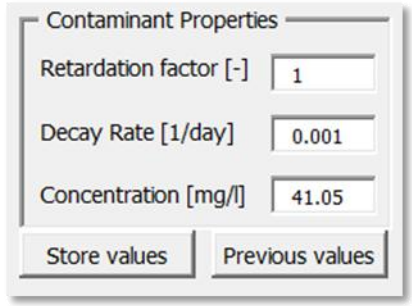

Figure 4.14: HPS GUI showing contaminant property inputs.

After changes are made, click on the 'Store values' button to save the inputs. Stored values can be used later by clicking 'Previous values' button.

4.2.2.4. Groundwater Velocity

The groundwater velocity or seepage velocity is calculated using Darcy's law. There are two options for calculating the groundwater velocity (Figure 4.15). The user can specify the magnitude of the local hydraulic gradient or it may be calculated. Check the 'Input Hydraulic Gradient Directly' box to enter a known or estimated gradient. Check the 'Calculate Seepage Velocity & Bearing' box for a model-calculated gradient. By providing the latitude, longitude and observed hydraulic head for three locations, the hydraulic gradient is calculated by the model. In these cases, the model will calculate both the magnitude and direction of the hydraulic gradient. After entering the data (lat, long and head), click on 'Run Groundwater Model' to obtain the hydraulic gradient, velocity magnitude, and direction.

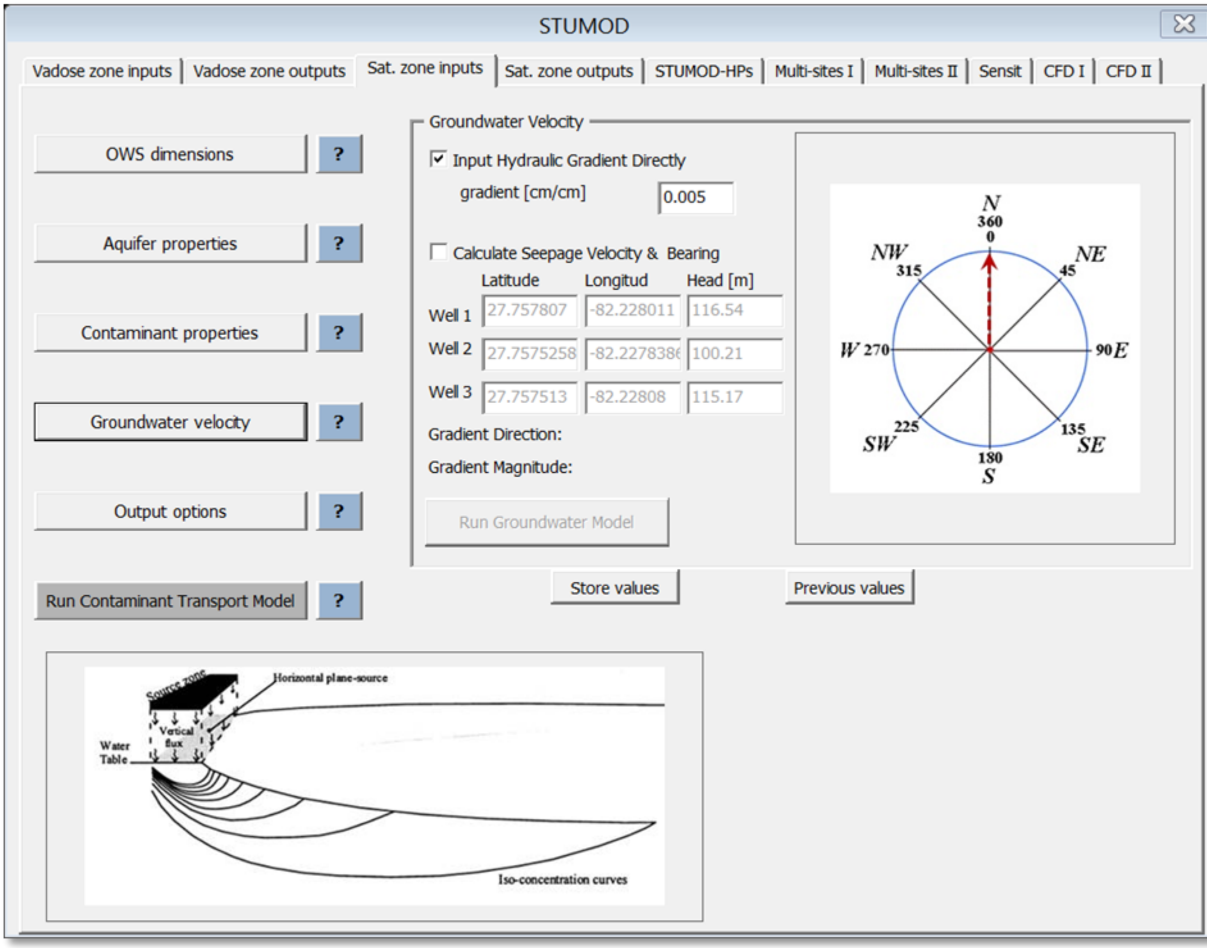

Figure 4.15: HPS GUI showing groundwater velocity inputs.

After changes are made, click on the 'Store values' button to save the inputs. Stored values can be used later by clicking 'Previous values' button.

4.2.2.5. Output Options

There are three options for computation and viewing the HPS outputs: 'Calculate Mass Flux', 'Calculate Concentration', and 'Y, Z Plume Cross Section' (Figure 4.16). The first option, 'Calculate Mass Flux' (in the left column of the GUI), and calculates mass flux through a vertical plane at user specified distance from the source. This option also calculates the centerline concentration. The distance can be directly input by choosing 'Input Distance to Target' or calculated by the model by choosing 'Calculate Distance'. For the direct input, the distance from the source in meters is entered. For the model calculated location the latitude and location of a point down gradient from the OWS is entered. The distance is calculated from the location data entered on the 'OWS Dimensions' menu (Figure 4.12) and the 'Output options' menu (Figure 4.16).

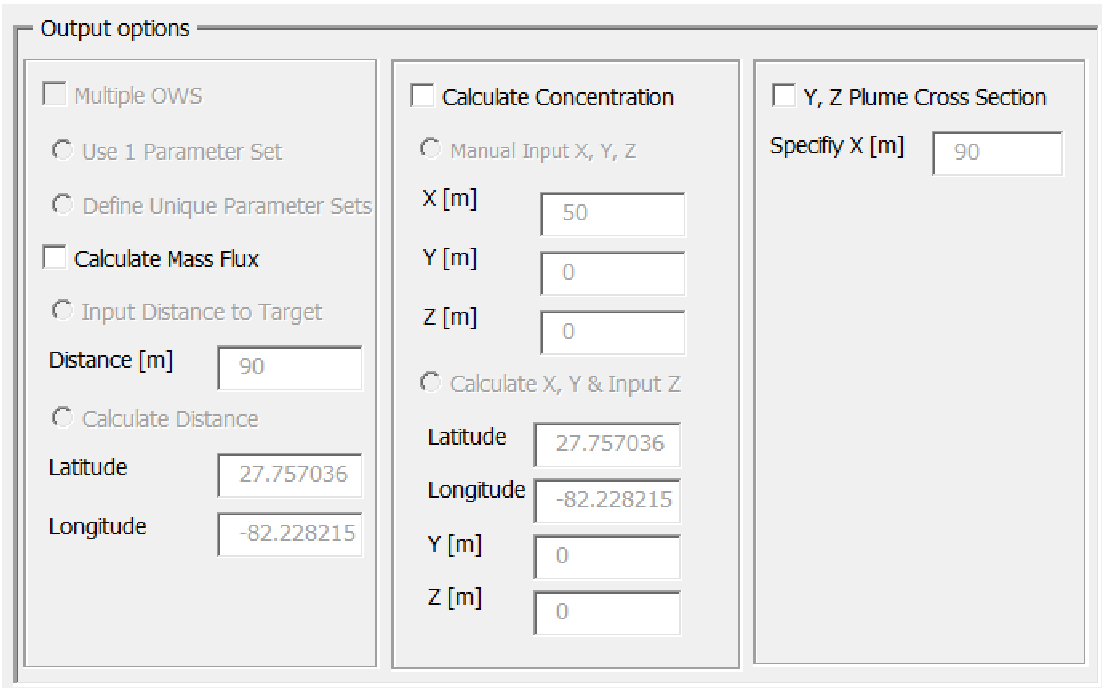

Figure 4.16: HPS GUI showing inputs for output options.

The second option, 'Calculate Concentration' (center column of the GUI) estimates only the centerline concentration. This option takes relatively short time run, but does not include the mass flux output.

The third option, 'Y, Z Plume Cross Section' (right column of GUI) provides the same information as the first option, but also generates an illustration of the vertical plume at the user specified down gradient location.

4.2.2.6 Running the HPS Module

After defining the input parameters listed in the main page (Figure 4.11), Select the 'Run Contaminant Transport Model' button to execute the module. To view the outputs, go to the 'Sat. zone outputs' tab. The saturated zone outputs are shown in Figure 4.17.

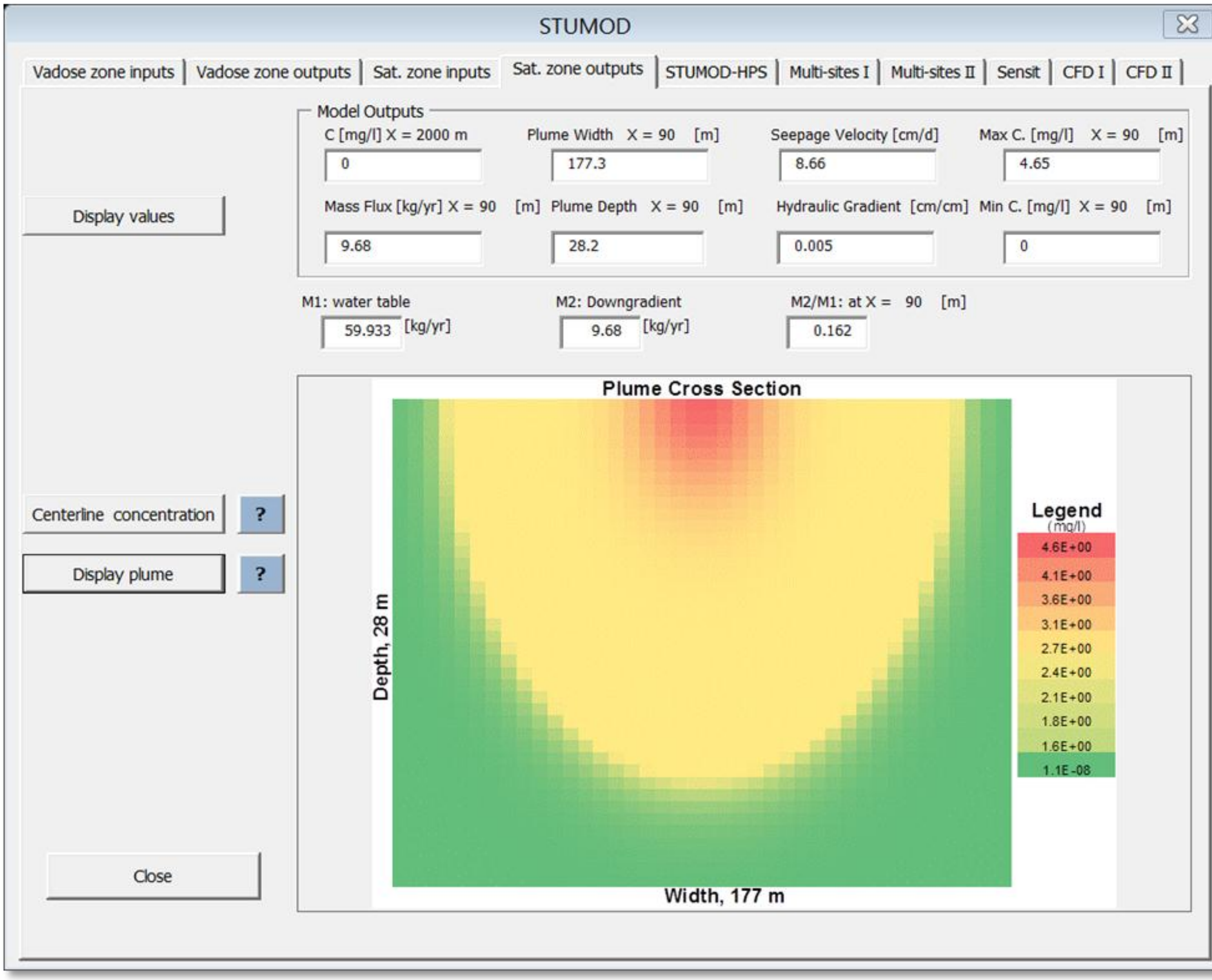

Figure 4.17: HPS GUI showing saturated zone outputs.

The 'Model Outputs' shown at the top of the GUI display shows values based on the output viewing options the user selects before running the model (Section 4.2.2.5). Model tabular outputs include plume width and depth, seepage velocity, hydraulic gradient, maximum and minimum concentrations at the user specified down gradient distance, the input mass flux at the water table and the output mass flux at the user specified down gradient distance and the percent of mass remaining.

The centerline concentration is displayed under the 'Model Graphical Outputs by clicking 'Centerline concentration' button on left side of the GUI. This will display the centerline concentration for the most recent run. The centerline concentration is valid regardless of the output viewing option selected. A vertical plume at the user specified distance is s displayed by clicking 'Display plume' button on the bottom left. The vertical plume output is valid only if the 'Y, Z Plume Cross Section' output option was chosen.

4.2.3 How to use the Combined STUMOD-HPS Module

The vadose zone module (STUMOD-FL) and the saturated zone module (HPS) were designed to run together generating both unsaturated and saturated zone outputs in this Combined STUMOD-HPS module. Users can generate outputs at the water table and at a down gradient distance in one model run. As with the individual modules, STUMOD-FL calculates boundary concentrations for the HPS module and HPS calculates mass loading and concentration at a distance the user specifies.

First, go to the STUMOD-FL input main page (Figure 4.2) and update all inputs (see Section 4.2.1). Next, go to the STUMOD-HPS tab and input a down gradient distance in the input box at the top left of the GUI (Figure 4.18). Click on 'Run STUMOD-HPS'. The vadose module will run first then proceed to HPS.

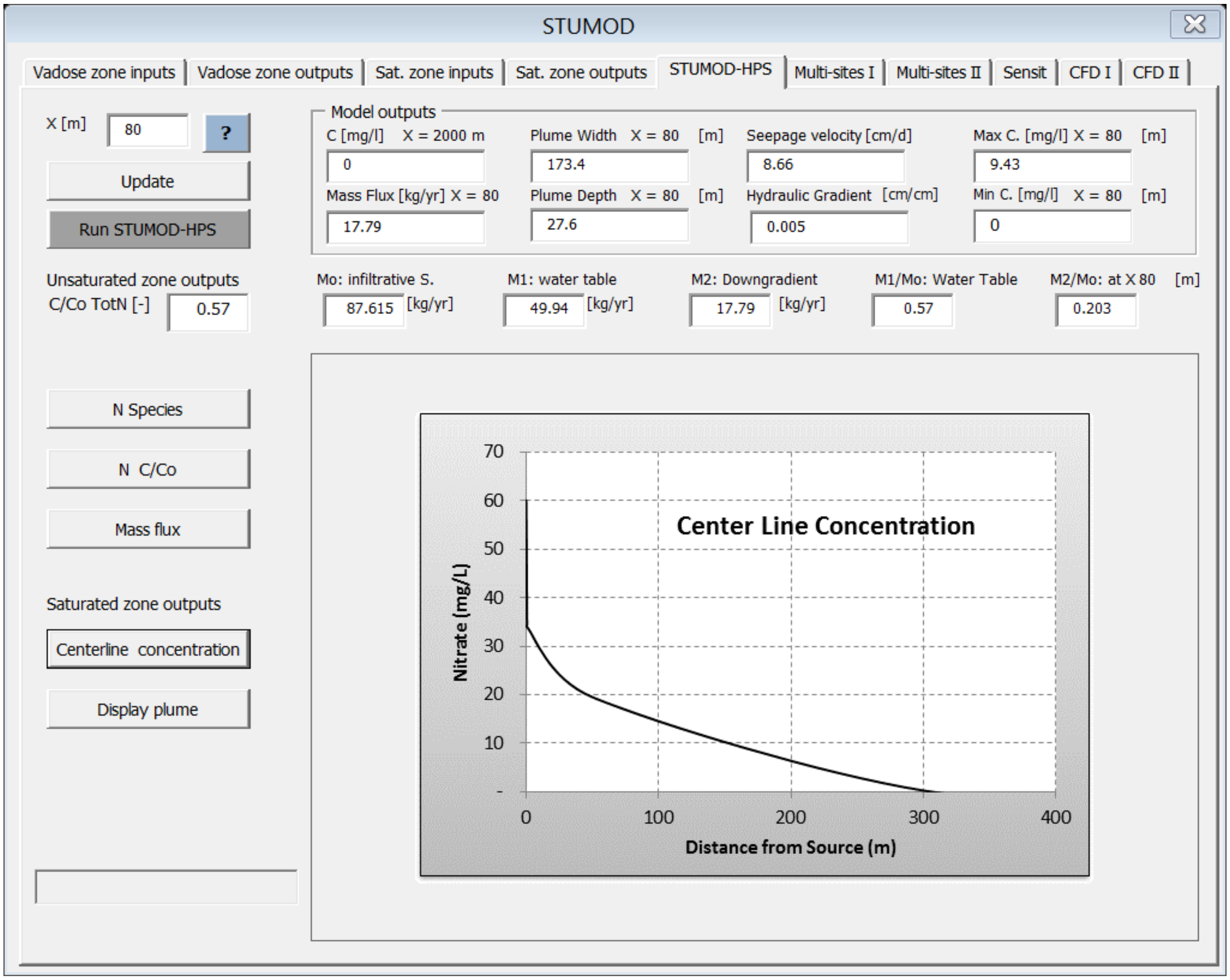

Figure 4.18: Combined STUMOD-HPS GUI showing inputs and outputs.

When the run is competed the input table in Figure 4.19 will appear with values populated from the vadose zone. These values will be used in the HPS module as the boundary concentrations. Users need to click 'update values' to send the values to the HPS. Users can change any of these inputs if needed.

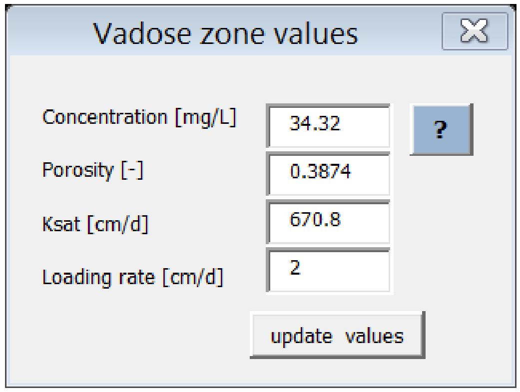

Figure 4.19: Combined STUMOD-HPS GUI showing vadose zone module outputs used for inputs to the saturated zone module.

The outputs shown in Figure 4.18 again include 'Model Outputs' on top and 'Model Graphical Outputs' at the bottom, but for both saturated and unsaturated zone outputs. Tabular outputs are displayed for the user specified down gradient distance, [X], including plume width, plume depth, maximum and minimum concentration, input mass flux at the water table, output mass flux, and percent of mass remaining. Values for seepage velocity and hydraulic gradient are also provided.

Graphical outputs for the unsaturated zone include concentration of ammonium, nitrate and total nitrogen, fraction of nitrogen remaining, and mass flux. Graphical outputs for the saturated zone include the centerline concentration starting from the infiltrative surface to distance [X]. Any graphical display will be shown by clicking on the associated buttons in the left column of the GUI.

4.2.4 How to use the Multiple Sites Module

This module calculates nitrogen mass flux [kg/yr] downstream at a specified distance from multiple sites. There are two separate modules, Multiple Sites I and II (see Section 3.3 and the Task D.14 report). Both modules include the option to evaluate unique parameter values at each site or lumped parameter values. For the lumped option, one parameter set is input by the user and applied uniformly across all the OWTS but the distance from each source to the receiving water body is varied. For the unique parameter option, the user can vary the parameter sets across all the OWTS including the distance from each source to the receiving water body.

4.2.4.1 Multiple Sites I

To begin, the user chooses the 'Multi-sites I' tab (Figure 4.20). From this GUI, click on 'view inputs' button and the input worksheet (MultipleSites_I) will be displayed. Users need to specify both saturated and unsaturated zone input parameters for each site. The unsaturated zone input parameters for each site are listed in columns C to BN with each site represented in a single row. Column A shows the site number. The soil type for each site can be selected from the dropdown menu in Column C. Based on the soil type selected, related unsaturated zone parameters are automatically populated with default values. The user can replace any default value. To restore the default values click on the 'Restore default values' button on top left of the worksheet.

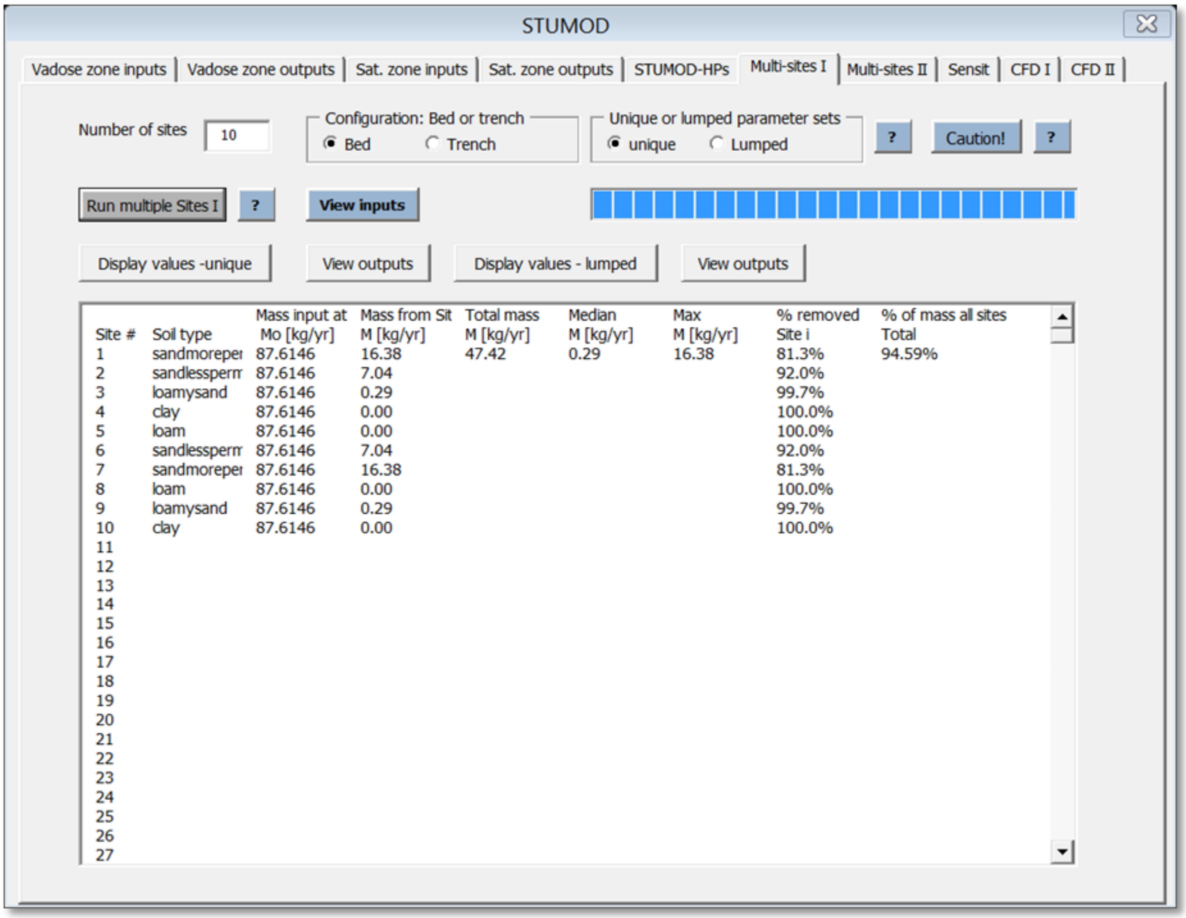

Figure 4.20: Multiple Sites I GUI showing module inputs and outputs.

Not all the parameters are automatically populated when choosing a soil type. There are a number of other parameter that should be populated by the user for each site include depth to water table (column BJ) and depth to water table options, either 'User Input WTD' or 'TD=WTD' in column BI.

The saturated zone inputs for parameters for each site are listed in column CF to DF. Important key inputs include hydraulic gradient (column CF), porosity (column CK) and saturated hydraulic conductivity (column CO). Porosity and saturated hydraulic conductivity are obtained from the unsaturated zone inputs (columns I &G). Concentration (column CR) is obtained from the unsaturated zone output (column BT). Other parameters include retardation (column CP), decay rate (column CQ) and dispersivity values (column CL to CN). Finally, an essential input is the distance to the point of interest down gradient of the STU from each site listed in column DD.

Once the inputs have been adjusted, click on the 'Back to GUI' button in Column A, Row 1 of the input worksheet. From the 'Multi-sites I' tab, click on either the 'Run-unique parameter set' or 'Run-lumped parameter set' button. After the module has run, table will be populated with mass flux from each site, total mass flux to the site, and fraction of mass removed for each site and for all sites (Figure 4.20). Click on the 'View outputs' button to review the outputs in the Multiplesites_I worksheet. Unsaturated zone outputs, including fraction of ammoniium, nitrate and total N remaining at the water table, and mass flux for each site used as input in the saturated zone module, are in columns BQ to CA. Saturated zone outputs are in colums DN and DU. To return to the Multi-sites I tab, click on the 'Back to GUI' button.

4.2.4.2 Multiple Sites II

This module calculates nitrogen mass flux [kg/yr] downstream at a specified distance from multiple sites just like the 'Multiple Site I', but it assumes known mass fluxes from the vadose zone to the water table. This approach requires relatively shorter run times because only the saturated zone module is executed. The number of sites should be specified. Large numbers of sites will require longer simulation times.

To begin, click on the 'Multi-sites II' tab. From the GUI, click on 'view inputs' button and the input worksheet (Multiple Sites_II) will be displayed. The concentration at the water table is a direct input for this module and the concentration input should be entered in column M. Saturated inputs should be reviewed and/or input similar to 'Multi-sites I'.

From the 'Multi-sites II' tab, click on either the 'Run-unique parameter set' or 'Run-lumped parameter set' button. After the module has run, again, outputs are provided for a user specifeid down gradinet location. Click on the 'View outputs' button to review the outputs in the MultipleSites_II worksheet. Saturated zone outputs are in colums DN and DU. To return to the Multi-sites II tab, click on the 'Back to GUI' button.

4.2.5 How to use the Sensitivity Module

A sensitivity analysis indicates which input parameters are critical to and which parameters have less influence on the final model output. For the Sensitivity module incorporated into STUMOD-FL (Section 3.4.1), a total of 8 parameters can be evaluated. Parameters are ranked based on relative change in output in response to change in inputs. This module is available for the unsaturated zone only and may take several hours to run.

To begin, go to the 'Sensit' tab (Figure F.21). Choose 'soil texture' and click on the 'Run Sensitivity' button. Click on 'view inputs' to go to the input table. The parameters that can be evaluated are (column headings are highlighted in yellow in the module): hydraulic loading rate (column D), porosity (column I), STE concentration (column M), nitrification rate (column Q), denitrification rate (column Z), temperature (column AD), sorption (column AE), and treatment depth (column AH). Users do not need change these inputs unless better information available.

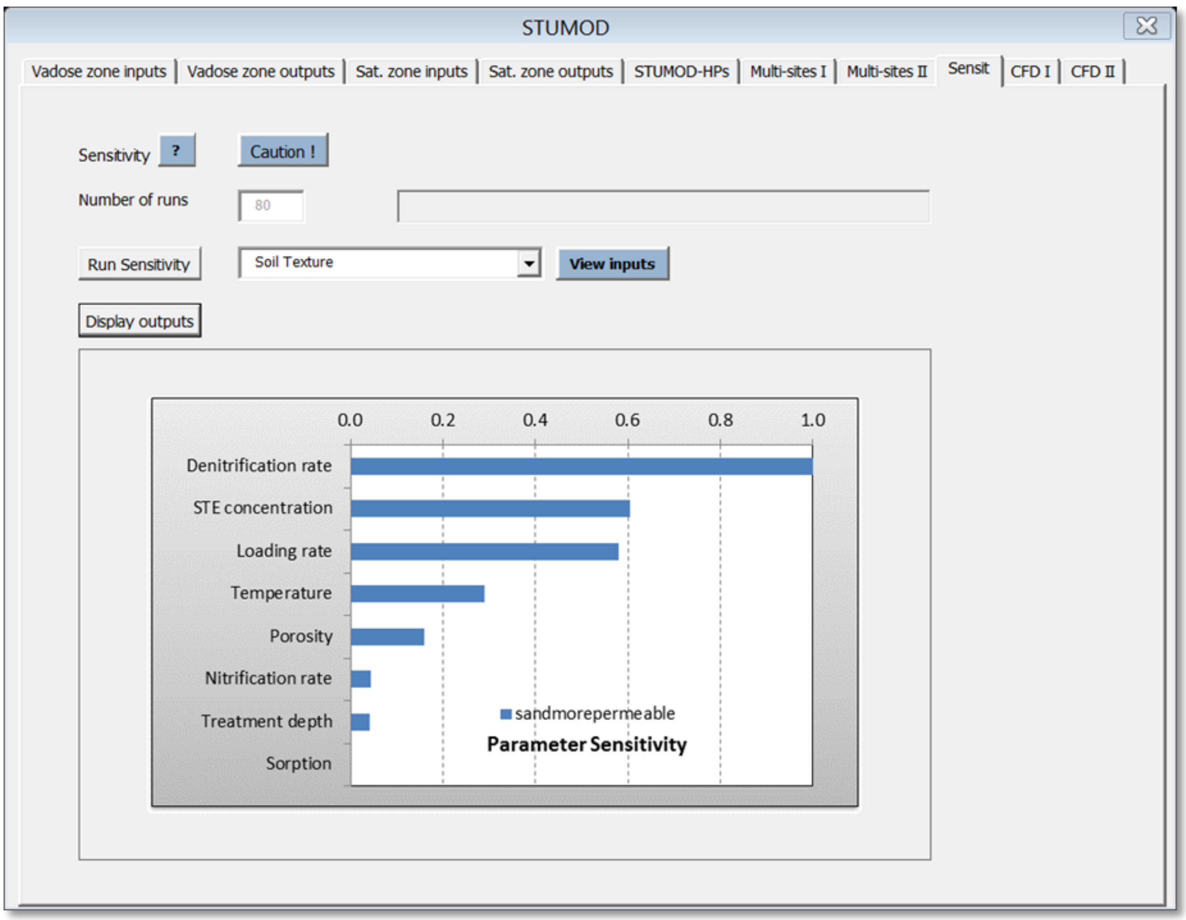

Figure 4.21: GUI showing sensitivity module inputs and outputs.

Click on the 'View inputs' button to review outputs (column BT) generated for each input parameter (see column BO to BV) based on input variations given in column BQ on the 'Sensitivity' worksheet. Corresponding outputs are given in Column BT. The standard deviation for the output corresponding to each to input parameter is given in cells BX7 to BX14. The normalized standard deviations for comparison are given in cells BY7 to BY14. To return to the GUI click on the 'Back to GUI' button. Click on the 'Display outputs' button to view the sensitivity results (Figure 4.21).

4.2.6 How to use the Uncertainty Module

The uncertainty module added to STUMOD-FL is based on a Monte Carlo simulation where the model is executed many times as input parameter value(s) are randomly generated within specified ranges (see Section 3.4.2). Statistical evaluation of the outputs is in the form of a cumulative frequency diagram (CFD). The CFD I module generates a CFD for the percent of nitrogen at the water table. The CFD II module generates a CFD for the percent of nitrogen at a down gradient distance.

4.2.6.1 CFD I

Select the 'CFD I' tab in the GUI (Figure 4.22). The CFD I module generates a CFD for the percent of nitrogen at the water table. For this vadose zone simulation, the input parameters that are varied are: saturated hydraulic conductivity (K_{sat}), residual soil moisture (Θ_r), saturated water content (Θ_s), van Genuchten fitting parameters alpha (α) and η, nitrification rate, denitrification rate, and soil temperature.

First, input the number of runs to be completed. Each run is synonymous with a single parameter variation to generate a Monte Carlo simulation output. As the number of simulations increases the robustness of the CFD is improved, but the run time increases. An insufficient number of runs will produce CFD plots that are non-unique, meaning that if the same number of simulations is repeated the shape of the subsequent CFD plot will be slightly different. During model development, it was observed that beyond 2000 simulations, the CFD plot did not change. If a large number of runs is selected (i.e., 1000 to 2000), it may take several hours to execute the model.

Select the soil type from the dropdown menu and then click on 'Run CFD I'. Click on the 'view inputs' button to view the inputs on the 'Uncertainty_I' worksheet. Click on the 'CFD output' button to display the simulation results (Figure 4.21). Outputs generated for each combination of input parameters are in column CQ to CU of the 'Uncertainty_I' worksheet.

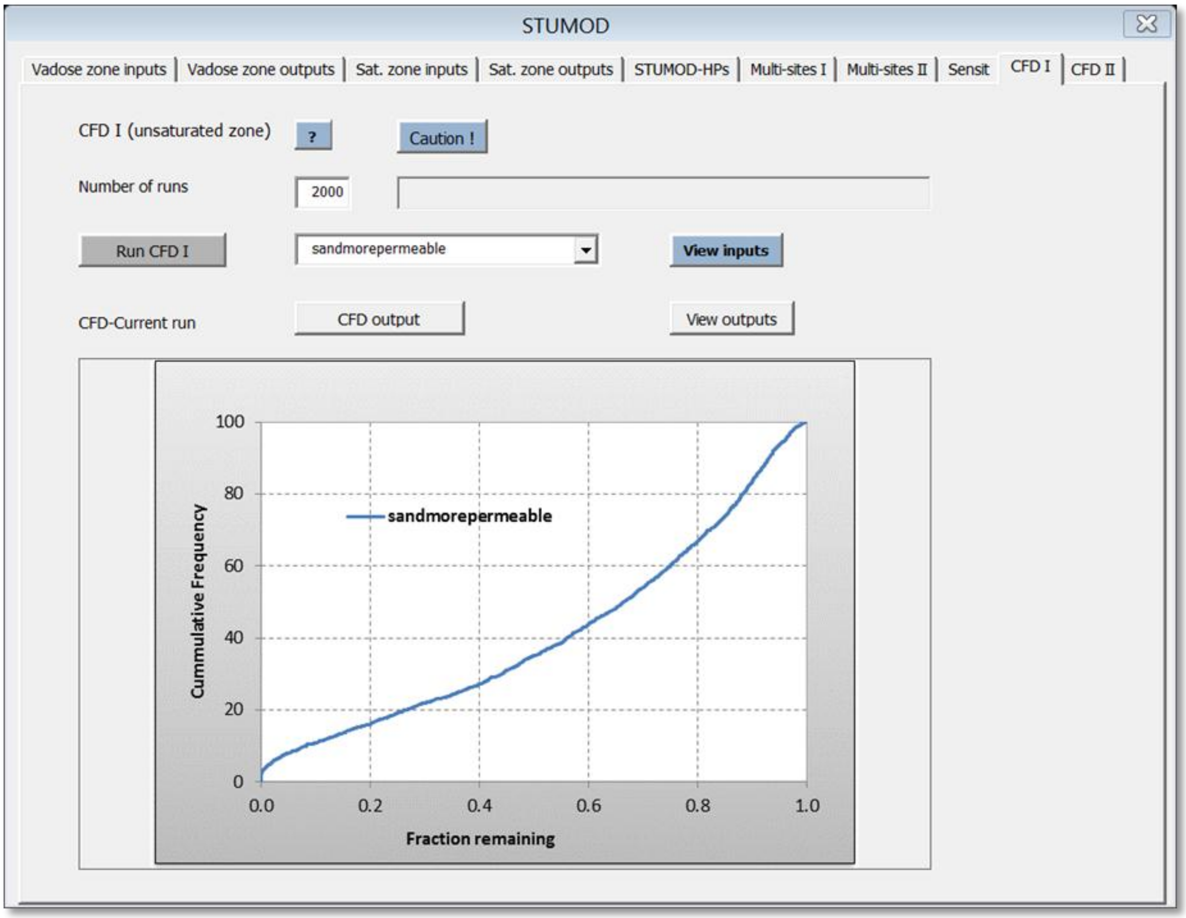

Figure 4.22: GUI showing CFD I module inputs and outputs.

4.2.6.2 CFD II

Select the 'CFD II' tab in the GUI (Figure 4.23). The CFD II module generates a CFD for the percent of nitrogen at a down gradient distance. For this saturated zone simulation, the input parameters that are varied are: porosity, saturated hydraulic conductivity (K_{sat}), dispersivity values, retardation, and denitrification rate.

As in the CFD I module, input the number of runs to be completed. Select the soil type from the dropdown menu and then click on 'Run CFD II'. Click on the 'view inputs' button to view the inputs on the 'Uncertainty_II' worksheet. Click on the 'CFD output' button to display the simulation results (Figure 4.23).

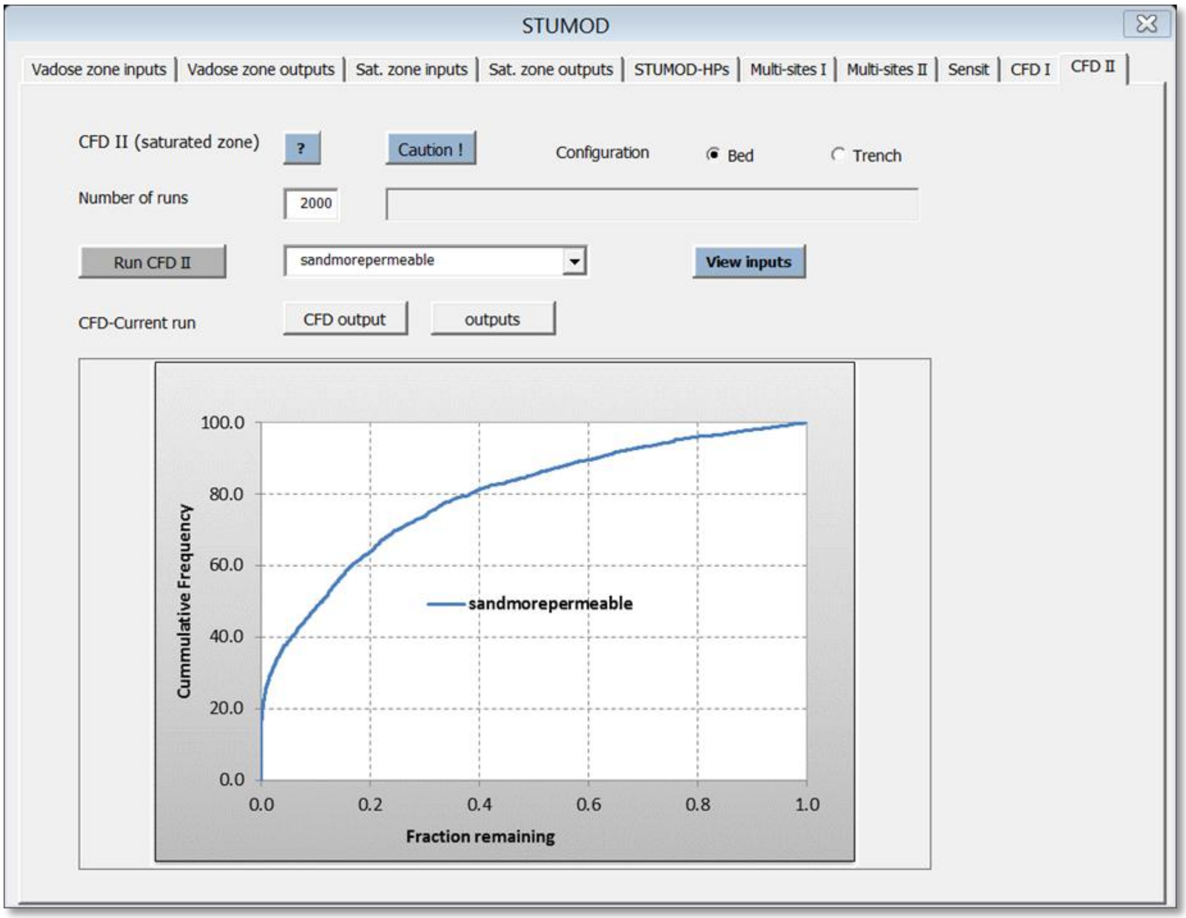

Figure 4.23: GUI showing CFD II module inputs and outputs.

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A. SOIL PARAMETER INFLUENCE

Table A.1
Summary of Estimated Default Parameters for STUMOD-FL based on Florida Soils

		Texture Fractions			Hydraulic Conductivity	Bulk Density	Residual Water Content (at 15 bars)	Saturated Water Content (at 3.5 cm)	Estimated van Genuchten Parameters	
Classification	**n**	**Sand**	**Silt**	**Clay**	K_{sat}	ρ	θ_r	θ_s	α	η
	-	%	%	%	cm/d	g/cm^3	cm^3/cm^3	cm^3/cm^3	1/cm	
Sand, more permeable*	1092	96.2	2.1	1.5	670.8	1.51	1.30	38.74	0.024	2.52
Sand, less permeable*	707	92.5	4.4	2.5	352.6	1.55	1.10	37.94	0.020	2.24
Clay	88	29.2	13.0	51.3	3.4	1.37	21.46	48.62	0.004	3.79
Clay Loam	9	38.0	30.5	31.4	7.4	1.44	15.24	46.21	0.009	1.76
Loam	23	45.0	35.4	20.1	17.0	1.36	10.35	42.14	0.012	1.63
Loamy Sand	460	84.8	8.1	7.2	164.9	1.57	3.64	37.78	0.020	1.76
Sandy Clay	56	51.9	7.6	38.8	14.2	1.55	15.41	41.64	0.004	3.45
Sandy Clay Loam	122	66.2	7.3	25.2	17.5	1.60	10.54	38.85	0.009	1.84
Sandy Loam	468	76.6	7.8	15.2	36.8	1.61	6.60	36.88	0.011	1.73
Silt	6	0.6	88.7	9.2	371.5	1.08	5.14	60.14	0.003	1.73
Silt Loam	9	5.7	82.0	15.8	185.3	1.01	5.78	60.54	0.003	1.69
Silty Clay**	0	-	-	-	-	-	-	-	-	-
Silty Clay Loam	5	5.8	65.6	28.9	7.4	1.13	27.71	59.86	0.009	1.51

* Sand soil series split into two groupings based on HCA, not textural classification. See Figure A.1.
** No complete data records in the Florida database for silty clay (<5ft deep).

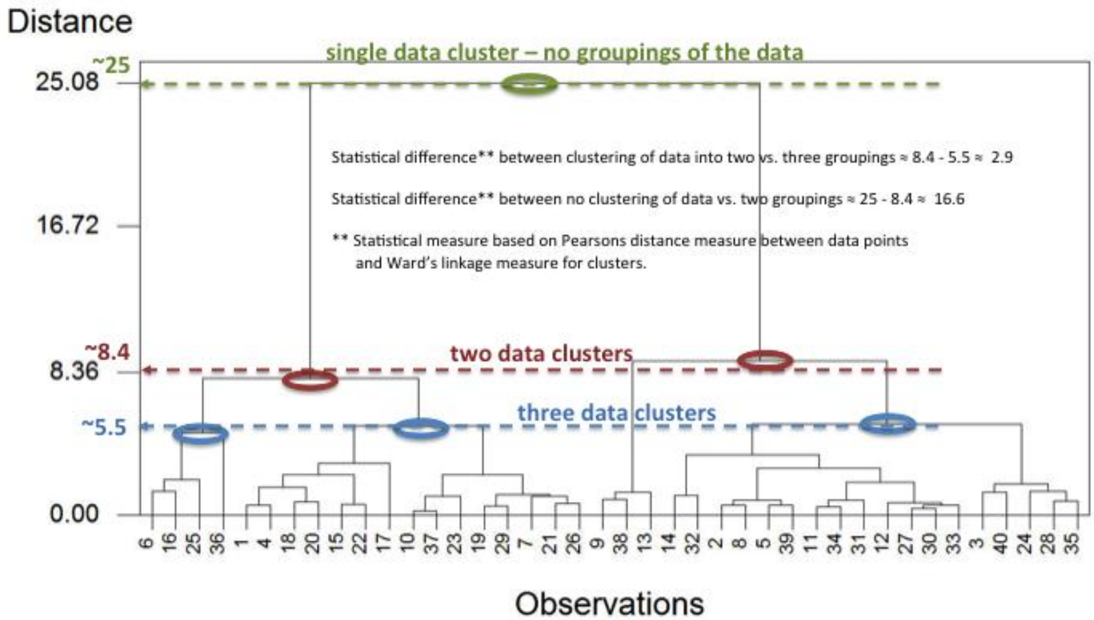

Figure A.1
Hierarchical cluster analysis dendrogram illustrating
two distinct subgroupings within sand soil series
(numbers on the x-axis are soil series identification - e.g., 1 = Adamsville)

Table A.2
Listing of Florida Sand Series Evaluated for Parameter Estimation

ID	Soil Series	# of Permits[1]	Ranking based on Permits	Areal Extent (acres)	Ranking within Total Florida Land Area	Ranking within Sand Series only	# of Records Used in Parameter Estimate
1	Adamsville	200	30	137,213	57	49	25
2	Albany	175	36	371,187	19	18	90
3	Alpin	175	37	249,585	33	29	39
4	Apopka	265	17	119,259	64	55	13
5	Arrendondo	235	22	199,867	39	34	26
6	Astatula	1136	4	493,691	8	8	38
7	Basinger	221	25	657,908	6	6	43
8	Blanton	461	10	475,052	10	10	69
9	Bonifay	226	24	234,420	34	30	27
10	Candler	2305	1	839,202	3	3	53
11	Eau Gallie	543	7	465,679	11	11	86
12	Felda	48	74	253,462	31	27	42
13	Floridana	NR[2]	>60	250,303	32	28	15
14	Holopaw	133	43	272,244	28	24	14
15	Immokalee	462	9	910,565	2	2	64
16	Lake	273	16	115,712	67	57	29
17	Lakeland	700	6	739,457	4	4	56
18	Leon	161	39	572,007	7	7	98
19	Malabar	121	47	344,605	20	19	62
--	Matlacha[2]	238	21	78,194	80	66	0
20	Millhopper	216	27	133,846	58	50	46
21	Myakka	1028	5	1,400,072	1	1	76
22	Oldsmar	254	20	297,163	23	21	63
23	Ortega	234	23	157,567	45	39	15
24	Otela	202	29	138,103	55	48	32
25	Paola	531	8	128,181	61	52	43
26	Pineda	184	33	421,044	16	16	63
27	Placid	24	102	267,790	29	25	20
28	Plummer	35	87	438,056	14	14	35
29	Pomello	265	18	216,530	36	32	55
30	Pomona	116	48	440,266	13	13	124
31	Riviera	159	40	491,995	9	9	44
32	Rutledge	23	103	303,268	21	20	11
33	Sapelo	66	66	273,399	27	23	83
34	Smyrna	350	13	714,008	5	5	61
35	Sparr	279	15	162,728	44	38	59
36	St Lucie	257	19	49,231	105	79	22

Table A.2
Listing of Florida Sand Series Evaluated for Parameter Estimation (cont.)

	Soil Series	# of Permits[1]	Ranking based on Permits	Areal Extent (acres)	Ranking within Total Florida Land Area	Ranking within Sand Series only	# of Records Used in Parameter Estimate
37	Tavares	1554	3	375,455	18	17	54
38	Troup	435	11	459,785	12	12	38
39	Wabasso	200	31	434,075	15	15	79
40	Zolfo	337	14	141,258	53	46	27

1 *Information on number of recent permits provided by FDOH (2012).*

2 *Excluded from further analysis – no data records reported in the Florida Soils Characterization Data Retrieval System.*

Table A.3
Listing of Florida Sandy Clay Loam Series Evaluated for Parameter Estimation

Soil Series	Series Textural Classification[1]	# of Permits[2]	Ranking based on Permits	Areal Extent (acres)	Ranking within Total Florida Land Area	# of Records Used in Parameter Estimate
Blanton	fine sand	461	10	475,052	10	1
Boca	sand	145	41	210,718	37	1
Bonifay	sand	226	24	234,420	34	2
Bonneau	loamy sand	111	49	147,125	51	9
Chaires	fine sand	11	132	221,332	35	5
Chobee	loamy fine sand	12	130	177,511	41	10
Dothan	sandy loam	193	32	297,410	22	10
Eau Gallie	sand	543	7	465,679	11	1
Esto	fine sandy loam	na	na	24,783	155	1
Felda	fine sand	48	74	253,462	31	1
Floridana	sand	17	118	250,303	32	4
Fuquay	sand	125	46	262,070	30	4
Kendrick	loamy sand	97	56	106,231	70	6
Lucy	loamy sand	70	62	133,837	59	5
Mascotte	fine sand	43	78	281,023	26	2
Maxton	loamy sand	2	215	1,739	307	1
Millhopper	sand	216	27	133,846	58	3
Orangeburg	loamy sand	207	28	282,002	25	15
Otela	fine sand	202	29	138,103	55	1
Pelham	loamy sand	93	57	393,382	17	4
Pineda	sand	184	33	421,044	16	1
Pomona	sand	116	48	440,266	13	8
Riviera	sand	159	40	491,995	9	2
Sapelo	fine sand	66	66	273,399	27	2
Sparr	fine sand	279	15	162,728	44	2
Surrency	loamy sand	1	238	284,796	24	3
Tooles	fine sand	2	221	144,731	52	1
Troup	fine sand	435	11	459,785	12	1
Wabasso	fine sand	200	31	434,075	15	6
Waccasassa	sandy clay loam	na	na	27,154	147	2
Winder	loamy sand	43	79	20,2519	38	8

[1] *Soil series textural classification is listed. However, only individual data records within the soil series classification listed as "sandy clay loam" were included in the evaluation.*

[2] *Information on number of recent permits provided by FDOH (2012).*